MonTec
Particle Optics Simulation Tools

Manuals:

- **INTERAC Modeling Environment**
- **Monte Carlo Simulation Program**

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1 Introduction

1.1 MonTec package overview

The MonTec Particle Optics Simulation Tools package supports the design and optimization of particle optical systems in which the impact of Coulomb interactions on the system performance is significant, e.g.:

- Electron- and ion-beam lithography systems
- Low-voltage scanning electron microscopes
- High brightness electron- or ion-sources

The MonTec package consists out of two separate, but tightly integrated, programs:

- The MS Excel based INTERAC program to define and analyze particle optical systems, and
- The FORTRAN based MC program to execute Monte Carlo simulations

INTERAC provides the means to define a particle optical system, to apply the analytical models for lens aberrations and particle interactions, to run and analyze the outcome of Monte Carlo simulations and to compare the outcome of the different theoretical approaches.

1.2 Manual overview

The introduction of this chapter describes the purpose and the design objectives of the MonTec Particle Optics Simulation Tools package and provides a high-level overview of the underlying theories. Chapter 2 explains how to get started. It covers the hardware and software requirements, the installation procedure, as well as a quick tour through the various INTERAC program features based on a sample session. Chapter 3 gives a full description of the INTERAC development environment and takes the reader through the functionality provided by the various worksheets. The working of the Monte Carlo simulation program MC is described in chapter 4.

The perspective chosen in chapter 4 is that of a stand-alone operation of the MC program. Some of this material is less relevant when running the MC program in conjunction with INTERAC, since INTERAC effectively acts as a shell around the MC program. When running the MC program from the INTERAC development environment, many tasks that should otherwise be performed by the user - such as the creation of the input files, the selection of proper values for the various modeling parameters as the sample size and number of seeds and the scheduling of jobs to run on the background through the workload mechanism - are taken care off automatically. Chapter 4, on the one hand, serves to provide insight the basic principles of the MC program which is also relevant for those users who operate the MC program through the INTERAC development environment and, on the other hand, explains how the MC operates as a standalone application, which is mainly relevant for those users who want to understand the details of how the INTERAC and MC programs work together or intend to use the MC

program on another computer system then a Windows based PC.

Chapter 5 reviews the relevant references to the public literature for further background information on the theory of the analytical models used for estimating the effect of Coulomb interactions, as well as the Monte Carlo simulation technique. A sample system is included as part of this manual which is used to demonstrate the working of both the INTERAC and the MC programs. The output file DEMO1.OUT of the sample session is reproduced in Appendix A. Appendix B contains a number of "screen shots" from the INTERAC program, which may serve to verify if INTERAC is running correctly on your system.

1.3   Theoretical basis

INTERAC provides an integrated capability to apply and compare the following alternative theoretical approaches to estimate the impact of Coulomb interactions in combination with lens aberrations:

- *Monte Carlo Simulation (MC) method:* This is a brute force numerical method in which *a* bunch of particles with randomly chosen initial coordinates, reflecting the properties of the beam in the vicinity of the source, is traced through a user defined system. The trajectories are determined by updating the positions and velocities of each particle at regular time intervals, taking the Coulomb repulsion experienced from all other particles in the bunch into account. Lenses and other optical elements can be specified and are modeled in the thin-lens approximation. The ray tracing can be repeated for a number of bunches, each starting with a different "seed" of initial conditions. The final coordinates, accumulated from all seeds, are processed in order to reduce the information to a limited number of characteristic quantities, such as the width of the energy distribution, the defocusing distance and the spatial broadening in the plane of best focus.

  INTERAC provides capabilities to automatically select values for MC parameters such as the sample size and the number of seeds; to create input files; to schedule batch jobs to run on the background and to extract and analyze the results stored in the output files of the MC program. The calculation of the particle trajectories by the MC program can be based on a full numerical algorithm or on the so-called FAST Monte Carlo Simulation (FMC) algorithm in which the analytical equations for two-particle interactions are utilized. The MC program allows for a uniform acceleration or deceleration of the beam in the beam sections in between the optical components (the so-called DRIFT spaces). See reference R-1 for further background information.

- *Analytical method* based on the so-called Extended Two-Particle (ETP) Approach: A set of analytical expressions to estimate the Boersch effect, the trajectory displacement effect and the defocusing and aberrations caused by space charge effects in a section of the beam. INTERAC breaks the system down into a number of beam sections, evaluates the impact of Coulomb interactions in each beam section and sums these contributions to determine the total effect on the system resolution at the target. The contributions of lens aberrations are included in thin-lens approximation. Different equations are incorporated for beam sections with a crossover and (nearly) parallel beam sections. The analytical equations apply to beam sections in drift space and ignore any acceleration or

deceleration of the beam. INTERAC includes the complete set of equations described in reference R-1 as well as the modifications for the trajectory displacement effect in broad beams described in ref R-2.

- *Slice method* based on a numerical integration of the analytical equations from the ETP-approach for a thin cylindrical slice of the beam; see reference R-1.The slice method is provides an adequate approximation in relative low density beams in which the deviations from the unperturbed trajectories are expected to be small. In terms of the ETP model these conditions correspond to the so-called Holtsmark and pencil-beam regimes. The slice method provides alternative estimates to the analytical method based on the same breakdown of the beam in beam sections. Unlike the analytical method, the slice method is capable to handle a uniform acceleration or deceleration of the beam in a beam section. The slice method also includes an algorithm to estimate the broadening of the beam under the influence of its own collective space charge force, using a laminar flow approximation. The purpose of this function is to validate that such broadening does NOT occur (since this would indicate that the beam operates at such high particle densities that the ETP model becomes inaccurate), rather than to estimate the actual space charge effects in this regime.

INTERAC provides the means to execute the three different methods from the same system description and to compare the results. The three different methods are complementary in many respects. MC exploits a brute force computation technique with a minimum number of underlying physical assumptions. It is therefore relatively slow, but accurate, provided that numerical procedures are carried out with sufficient caution. The analytical and slice method are based on analytical equations and provides immediate results since little computation is involved. These results may be less accurate due to the approximations underlying the analytical model, but provide a direct insight in the dependencies on the experimental parameters.

The reader is referred to chapter 5 for references to the literature on the theoretical framework used by INTERAC. Reference R-1 provides a full description of the alternative approaches to calculate the impact of Coulomb interactions in particle optical systems. The analytical equations derived in this publication on the basis of the so-called Extended Two Particle approach are used by INTERAC to calculate the Boersch effect, the trajectory displacement as well as the space charge

The theory outlined in reference R-1 was developed for probe forming systems, such as electron and ion scanning microscopes and Gaussian or shaped beam lithography systems. Fit-functions are used within the theory to express part of the numerical output into explicit analytical prescriptions. These functions were found to become inaccurate for the relatively wide beams typically used in the more recently developed projection type lithography systems. New fit-functions are presented in reference R-2 which extend the applicability of the theory to the wide beams and doublet configurations used in projection systems.

Reference R-2 also describes some modifications to the Monte Carlo program to account for the first order space charge magnification effect. This effect could be ignored for the relatively small spots of Gaussian and shaped beam systems, but would yield a significant overestimation of the trajectory displacement effect - assumed to be identical to the remaining blur after refocusing - for the wide images used in projection type of systems.

In the default setting INTERAC employs the full set of equations described in reference R-1, taking the modifications provided by reference R-2 for the trajectory displacement effect into account. The default setting can be changed to base all calculations on the original equations of reference R-1, ignoring the modifications of R-2, to investigate the difference between the two sets of equations for the trajectory displacement effect.

1.4 MonTec package design objectives

The MonTec Particle Optics Simulation Tools package has been designed to meet the following objectives:

- Provide an *Integrated modeling environment*: INTERAC provides an interactive user interface to specify the properties of a particle optical system consisting out of a particle source, followed by a succession of particle optical components - such as lenses, quadrupoles, deflectors and apertures – separated by drift spaces or spaces where the beam is linearly accelerated or decelerated. INTERAC provides a plot of the system as it is defined, showing the various optical components and the beam built-up from the first-order primary rays. The system plot is generated dynamically, meaning that any changes made by the user to the input data are directly reflected in the system plot. The system description defined this way is used by INTERAC to calculate first order properties of the beam, the geometrical and chromatic aberrations and the impact of Coulomb interactions. The same system description is used to execute both the analytical and slice-method calculations and to generate the input files for the corresponding MC simulation. The results of the MC simulation can be imported to allow a direct comparison of the results obtained with the analytical approach, the slice method and the MC simulation.

- Provide *automatic parameter selection for analytical and Monte Carlo calculations*. Given the system specification, INTERAC automatically determines the input parameters for the analytical and slice method calculations based on an analysis of the location of beam crossovers, the location of the image planes conjugated to the source and the target and the transverse magnifications from these planes to the source and target respectively. These automatically generated input parameters for the analytical and slice method can be overwritten by the user if desired. For the Monte Carlo simulations, INTERAC provides a facility to automatically set some of the key MC model parameters such as the sample size NSAM and number of seeds NSEED. For this, INTERAC evaluates the sample length relative to the lateral dimensions of the beam, assuring that some user-specified critical ratios are met. Based on the selected MC input data, INTERAC also estimates the run time of

the corresponding MC simulation. These facilities provide the means to balance the run-time and the expected accuracy of the MC simulation prior to execution. The automatic parameter settings provided by INTERAC allow the users to carry out analytical calculations and MC simulations without the need to explore the details of the underlying modeling concepts.

- Provide *graphical tools to inspect Monte Carlo results*. The various output files generated by the Monte Carlo programming - containing the general output data, the energy distributions, the spatial distributions in selected reference planes, the lateral particle positions in selected reference planes and the complete phase-space co-ordinates of all particles near the target – can be imported by INTERAC for subsequent analysis. INTERAC automatically create plots of the energy and spatial distributions, the lateral particle positions in the reference planes, as well as various cross-section of the phase space co-ordinates near the target. INTERAC thereby provides the means to inspect all MC results in full detail and replaces the program MCPLOT provided in the previous release of the MonTec package.

- Provide *data management facilities to design and administrate computer experiments*: INTERAC associates each case with a unique run-number and employs series IDs to allow the user to specify groups of runs. Each run corresponds to a unique user-specified set of MC input and output file names. Various file manipulations and data storage tasks can be executed for a selected series of MC runs through a single instruction by the user. Furthermore, INTERAC has incorporated the means to compare and plot the results of different runs to investigate the dependency on system as well as model parameters.

- Provide *flexibility while assuring maintainability*: INTERAC has been designed to provide rich functionality and extensive flexibility. The user can specify various series of runs to analyze a particle optical system under different experimental conditions, apply alternative theoretical approaches, store the corresponding results and create customized plots to analyze trends. The user may also change various modeling, data-management and plotting parameters to tailor INTERAC to its specific needs. In order to assure that INTERAC can be properly maintained, default settings can be retrieved on individual basis or for all parameters as a whole. INTERAC includes various spreadsheet management functions to restore default settings and clear user data.

Overall, INTERAC has been designed to create a modeling environment that is both powerful and easy to use. INTERAC provides the means to model particle beam systems quickly without the need for a detailed understanding of the underlying theory.

2 Getting started

2.1 Hardware and software requirements

INTERAC runs under Microsoft Excel 97, 2000, 2002 or higher and uses 30 MB of hard disk space or less, the exact figure depending on the amount of data loaded in to the program.

The MC program requires less than 1 MB of hard disk space for the executable, but the input / output files can be large depending on the number of particles in the simulation and whether all particle positions and/or co-ordinates are stored as output (*.POS and *.COR files). The dynamic memory requirement depends on the settings of the MONTEC.INC file for the maximum number of particles in the sample (MSAM) and the maximum total number of particles at the target (MTOT). The program MC has been compiled with MSAM = MTOT = 750,000. When using MC with the maximum total number of particles (NTOT) of 750,000, it will require about 350 MB of dynamic memory space.

INTERAC works best with a high resolution screen of at least 1280 x 1024 pixels. At lower resolutions, it may be difficult to get the full width of some of the worksheets on your screen with acceptable readability. A zoom-button is included on the top of each worksheet to adapt the screen size to the specific resolution of your monitor.

2.2 Installation

The installation and configuration of the MonTec Particle Optics Simulation Tools package is straightforward and consists out of the following steps:

- Create a directory structure on your hard disk and copy the MonTec program files. The simplest way to do this is by copying the complete file structure of the MonTec Program Package CD ROM to the hard drive of your PC. It is recommended to copy the file structure to the root directory of a hard drive, for example, the C: drive. When you would copy the default MonTec file structure to the root directory of the C: drive, you should have the following directories and files:

Directory	Reference:	Contained files (at installation):
C:\Montec\Run	*'INTERAC and MC run files directory'*	INTERAC.XLS Excel file. MC run files MC.EXE, RUN.BAT, DELINE.EXE and MAKEIOF.EXE.
C:\Montec\In\Demo	*'MC demo input files directory'*	All demo *.DAT and *.SYS files provided with the package.
C:\Montec\Out\Demo	*'MC demo output files directory'*	None until you have run the demo input files with INTERAC/MC.
C:\Montec\In	*'MC user input files directory'*	None until you have created your MC input files with INTERAC.
C:\Montec\Out	*'MC user output files directory'*	None until you have run your MC input files with INTERAC/MC.
C:\Montec\Doc	*'INTERAC documentation directory'*	MonTec_Manuals.pdf (this file) and MonTec_Brochure.pps documentation files.

Alternatively, you could also store all run and input/output files in a single directory (e.g.

\....\Montec). If you decide to take this approach, please bear in mind that every MC run uses two input files and creates four output files. It may therefore become somewhat of a challenge after a while to maintain the overview when you store all files in one directory.

NOTE: When using separate directories for the MC run files, the MC input and MC output files (as in the default setting shown in the table), you should avoid the use long directory names (such as for example *'C:\ProgramFiles\ParticleOptics\MonTec\Run\MySystem\In'*). INTERAC uses a so-called *'Execution command line'* (as specified in the second section of the *'Dashboard'* worksheet) to start MC and assign the input/output files. Long directory names may cause the command line to become too long (that is over 100 characters) which may cause errors. Hence, the recommendation to place the MonTec file structure at a root directory.

The core MonTec program files are INTERAC.XLS and MC.EXE. In case you are interested to understand what the other executable files in the Mc run files directory are doing, here is a brief overview.

File	Function*:
MC.EXE	Monte Carlo Executable
RUN.BAT	BAT file that INTERAC uses to start the MC program and specify the input/output file names through the parameters added to the RUN command, e.g.: C> RUN MC DEMO1 DEMO Starts MC.EXE and specifies DEMO1.DAT and DEMO1.SYS as input files and DEMO1.OUT, DEMO1.COR, DEMO1.EDI, DEMO1.SDI and DEMO1.POS as output files
MAKEIOF.EXE	Utility used by RUN.BAT to create the input/output file list
DELINE.EXE	Utility used by RUN.BAT to delete the first line of the WORKLD.BAT file to assure that the next run is executed in the next call to WORKLD

(*) Functions are described to indicate the purpose of these programs/utilities: Don't worry about what these files do, INTERAC does it all for you.

- Start Excel and open INTERAC.XLS. Excel may ask whether you want to <u>D</u>isable or <u>E</u>nable the macros contained in INTERAC.XLS. Select <u>E</u>nable. When you are running INTERAC for the first time it will show a so-called activation form in which you are asked to enter the installation code provided with the package, as well as your name and the name of your organization. The INTERAC Macro procedures will not run until the correct activation code has been entered. INTERAC will save the activation code and will not ask for this information again as long as it runs in the same system environment. At each start-up, INTERAC also inspects a number system and program properties (such as the Excel version, the regional settings and the screen resolution) and may prompt remarks when these settings are deviating from the INTERAC required settings. If the settings are OK and the correct installation code has been entered, INTERAC will show the opening splash-screen for a few seconds and select the *Dashboard* worksheet.

- In the worksheet *'Dashboard'*, you should verify if the *'MC run files directory'*, the '*MC input files directory*' and the '*MC output files directory*' specified in the top section of the worksheets

corresponds to the MonTec directory structure. No changes are required when you have taken over the default configuration listed in the table above. When you have used a different directory structure you need to modified the directories and/or drives by editing the corresponding fields, or, alternatively, by pressing the "Browse" button on the right hand side of the screen and selecting a directory on the folders window. In case you want to store the MC input and output files in the same directory as the run files directory, press the button '*Same as run files*'.

2.3 Quick tour and sample session

2.3.1 Worksheets overview
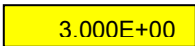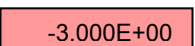
The INTERAC workbook consists of 16 user worksheets, which can - in the regular display mode - be selected through the worksheet tabs on the bottom of the screen. The table below provides an overview of the different worksheets and their main function.

Worksheet:	Main Function:
Dashboard	Central area from which most program functions are controlled
System	Interactive environment to enter, review and modify all system quantities and to specify the model parameters for the different calculation methods. The system plot in the top-section shows the beam optical components, beam geometry, principal rays based on the data shown in the sections below. Various sections are included to specify the MC method and the analytical/slice method parameters.
Section	Interactive environment to analyze the results of the analytical and slice method for an individual beam section.
MC_in	Input data from the DAT and SYS files for the selected run
MC_out	Output data from the OUT file for the selected run and comparison with the analytical/slice method results.
MC_edi	Output data on the energy distribution from the EDI file for the selected run
MC_sdi	Output data on the spatial distribution from the SDI file for the selected run
MC_pos	Output data on the particle positions from the POS file for the selected run
MC_cor	Output data on the particle co-ordinates from the COR file for the selected run
PlotDis	Plots of the energy and spatial distribution for the selected run
PlotPos	Plots of the final particle positions in the reference plane(s) for the selected run
PlotCor	Plots of the final particle co-ordinates in various "position" and "velocity" views
Runs	Specification of runs in terms of input and output files identifiers
Results	Summary of key input and output data of the MC, analytical and slice method for all runs
PlotRuns1	User specified plots of the selected results from the worksheet '*Results*' using a labeled horizontal axis (e.g. to compare results for various non-related MC parameter settings)
PlotRuns2	User specified plots of the selected results from the worksheet '*Results*' using a continuous horizontal axis (e.g. to compare results for different settings of a single MC parameter)
About	Contains documentation and other general program information
Settings	Program settings on e.g. the main model parameters, numerical and physical constants, Excel calculation mode, and array sizes.

2.3.2 Spreadsheet conventions and display-controls

Most worksheets contain a mixture of headings, guidelines, input cells, output areas, graphs and macro-controls, which together constitute the user interface. Before exploring the individual

worksheets in more detail, it is helpful to understand the meaning of the various cell- and font-colors and the working of some of the controls used to tailor the worksheet views.

Yellow cells with boldface characters (e.g. ☐) indicate areas where the user can input data or select options. Yellow cells with regular font, that is non-boldface characters (e.g. 3.000E+00) represent data automatically selected by INTERAC, that can be overwritten by the user. Data can be entered by selecting a yellow cell with the mouse and entering the data. For some cells input data can be selected from a dropdown list which appears the cell is selected. Yellow cells turn light read (e.g. -3.000E+00) when the data entered deviates from the default setting for that cell and signal red with a white boldface text font (e.g. **-3.000E+00**) when the entered data is outside the range of valid entries.

Grey buttons (e.g. **Run job**) represent macro controls that can be activated by the user by pointing and clicking with the mouse. Some worksheets contain checkboxes and radio buttons through which the user can select specific options.

Some navigation controls are repeated in the top-bar of each worksheet. One such a control is the so-called '*Full Screen Mode'* switch (Full Screen On/Off). By clicking on this control the user can toggle the '*Full Screen Mode'* on and off, with the following effect:

Display mode:	Operation:
Full Screen On	This mode provides the large working-screen display window by removing the standard Excel bars (toolbars, tab sheet bars, etc.) from the bottom and the top of the screen, as well as the slide bar normally on the right side of the screen. INTERAC provides alternative "Sheet Tabs" for the navigation between worksheets on the top of the screen
Full Screen Off	Regular user specified Excel view

Most worksheets have a '*Expand'* and '*Collapse'* control (Expand and Collapse) in the top line to show or hide part of the screen. The *System* and *Section* worksheets consist out of various sections (or areas) which can be shown or hidden on an individual basis through the '*Expand'* and '*Collapse'* buttons in the headings of each section. All areas can be expanded or collapsed in one go through the '*Expand all areas'* and '*Collapse all areas'* (Expand all areas and Collapse all areas) buttons on the top.

Appendix B contains a number of "screen shots" from the INTERAC program, which may serve to verify if INTERAC is running correctly on your system.

2.3.3 Demo system

Go to the worksheet '*Systems'*. In the default setting, one sees in the top chart (entitled '*System Plot'*) a schematic representation of a electron beam projection lithography system resembling the properties of the SCALPEL Proof of Concept (See reference R-2 for a summary or the original data in S.D. Berger et al.,J. Vac. Sci. Technol. B 9. 1996 (1991) or S.D. Berger et al., Proc. SPIE 2322, 434 (1994). If needed press on the 'Load demo system' button (**Load demo system**) on the top left of the *System*

worksheet to restore the demo system. The figure below shows the schematics of such a charged particle projector lithography system.
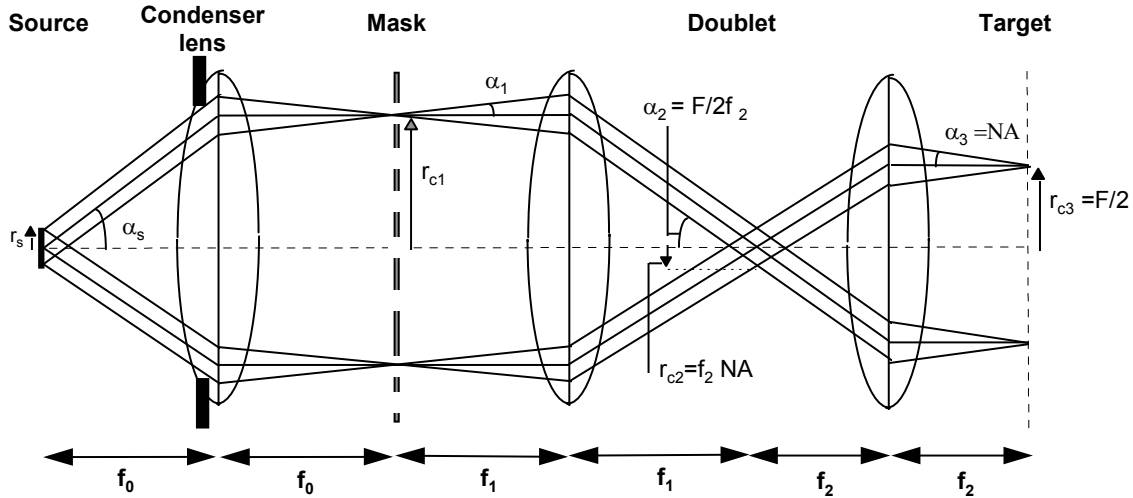
The system consist out off five beam sections. Beam section 1 runs from the source to the condenser lens and condenser aperture, located at the same axial position in the model representation. Section 2 runs condenser lens to reticle. Section 3 from the reticle to the first lens from the doublet. The 4th beam section contains the beam segment with a crossover in between the two lenses of the doublet. The 5th and final beam section runs from the second doublet lens to the target. See reference R-2 for further details and an explanation of the symbols in the figure.

Press on the *'Set-up screen for system input'* (**Set-up screen for system input**) control to see the system plot and the systems specification areas in one view. If needed press the *'Collapse'* buttons in the table sections entitled *'Quadrupoles'* and *'Deflectors'* of the *'Optical Components and Drift Sections'* area. To see the effect of changing the data, select the cell in which the focal distance of the condenser lens is specified, which is the entry in the 2nd beam section where at the row with the identifier F. The default entry in the demo system is 0.16 m. You can change the value by typing another value, e.g. 0.12 m. Observe that the change is immediately reflected in the system plot. Another way to change the value in a yellow cell is to select the cell and then press the *'Increase abs', or 'decrease abs',* *'Increase %' , o*r *'decrease %'* buttons (Increase abs , Decrease abs , etc.) the top-right hand side of the *System* worksheet, which will change the cell entry with the absolute step value or relative % value, specified next to these buttons. Set the entry back to the value 0.16 m.

Press the *'Expand all areas'* button in the top left of the worksheet. You may want to scroll through the remainder of the sections in the *'System'* worksheet, which are briefly described in the table below:

Worksheet *'System'* section title:	Functionality:
Scaling & Optical Properties	Specifies the scaling of the *'System Plot'* and lists the optical properties of the system as derived by INTERAC
Ray Tracing & Plot Parameters	User control area to set the ray-tracing as well as some plot parameters of the *'System Plot'*
Source Properties	System input for the source properties

Worksheet *'System'* section title:	Functionality:
Optical Components and Drift Sections	System input for the optical components and drift/acceleration/deceleration spaces in between the optical components
Monte Carlo Simulation Parameters	Input / calculation of the optimum MC model parameters
Analytical Model Parameters for Coulomb interaction Effects	Input parameters for the analytical and slice calculation by beam section. INTERAC automatically derives this data from the system input data, but the user may overwrite this data
Analytical Results for Coulomb interaction Effects	Results of the analytical and slice method calculations and listing of the selected results from these methods for the total system calculation
Comparison of Analytical Results from Different Methods and by Beam Section	Results of the analytical and slice method calculations and listing of the selected results from these methods for the total system calculation
Comparison of Analytical Results from Different Methods and by Beam Section	Set of charts to compare the results obtained with the different methods as well as the contribution of the different beam sections relative to the total effect at the target
Analytical Results for Total Energy Spread	Results for the total energy spread at the target obtained by adding the energy broadening caused by the Boersch effect to the source energy spread (specified as system input)
Analytical Results for Total Probe Size	Total system resolution and breakdown in Coulomb interaction effects, geometrical spot size and lens aberrations.
User Specified Curves	Facility to evaluate the Coulomb interaction effects and total probe size contributions as function of a range of values for one or more system input parameters specified by the user and set of charts to plot the results
Output tables	Listing of the results obtained for the *'User Specified Curves'*

2.3.4 Executing a Monte Carlo simulation of the DEMO system
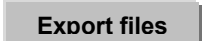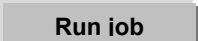
Select the worksheet *'Dashboard'* and enter 1 as the *'Selected run no.'.* The MC input file names given in the section *'Input and Output File Names For Selected Run'* should now be DEMO1.DAT and DEMO1.SYS. All indicated file names are derived from the Data run identifier and System file identifier, which are for the selected run 1 both equal to 'DEMO1' as indicated in top section of the *'Dashboard'*.

The file identifiers are specified in the worksheet *'Runs'. G*o to the worksheet *'Runs'* and have a look at the various demo runs defined in this table. In the default setting the following runs and run series are specified:

Run	Series ID	System parameters	MC parameters
1	Default	I(uA)=10, V(kV)=100	automatic, DRIFT2
2-8	DEMO-TS	I(uA)=100, V(kV)=100	NSAM=200-20000; NSEED=100-1, DRIFT2
9-15	DEMO-IS	I(uA)=1-200, V(kV)=100	automatic, DRIFT2
16-21	DEMO-VS	I(uA)=10, V(kV)=5 - 200	automatic, DRIFT2
22-24	DEMO-IS-D1	I(uA)=1, 10, 100, V(kV)=100	automatic, DRIFT1
25-30	Systems	Various systems included for demonstration purposes.	automatic, DRIFT2

Go back to the worksheet *'Dashboard'* and do the following to carry out the Monte Carlo simulation for this system:

- Make sure that 1 is the selected run no. and that the check-boxes in the left part of the *'Monte Carlo Simulation'* section are checked (instructing INTERAC to copy system data to MC_in and to export both the MC SYS and the MC DAT file).

- Press *'Export files'* (**Export files**) in the *'Monte Carlo Simulation'* section. If the DEMO1.SYS and DEMO1.DAT file already exist in the MC input files directory, INTERAC will ask if you want to overwrite these files. In that case, press YES. You may want to press *'Edit files'* (**Edit files**) *to* see how the exported files look like. This control should open two Notepad windows containing the DEMO1.SYS and DEMO1.DAT file respectively (You may specify a different editor than Notepad in the worksheet 'Settings'). Close both Notepad windows.

- Now press *'Run job'* (**Run job**) in *'Monte Carlo Simulation'* section. You should now see a command prompt (DOS) window with the MC screen. On a 3.0 GHz Pentium IV machine with running Excel 2002 under Windows XP, the program should finishes in about 10 sec.

- No press *'Import checked files'* (**Import "checked" files**) in the *'Data analysis section'* of the *'Dashboard'* worksheet (Make sure that all files are checked in the left area). You should now see messages that all files are read, analyzed and stored successively. If everything works properly, there shouldn't be any error messages in the *'Dashboard', 'System'* or the *'Section'* worksheets.

Congratulations, you have just carried out some of the core INTERAC functions: You have defined a particle optics system, exported the MC input files, executed an MC simulation and imported the results. The analytical and slice calculations have been performed automatically when INTERAC imported the MC.DAT and MC.SYS files. Press the *'Store data for selected run'* button in the *'Data Storage to Worksheet Results'* section of the *'Dashboard'* worksheet. You may now wish to inspect the results of the MC run and the corresponding analytical calculation. Have a look at the worksheets *MC_in, MC_out, PlotDis, PlotPos* and *PlotCor.*

2.3.5 Exploring individual beam sections

Go to the worksheet *'Section'*. In the default setting, one sees in the top chart (entitled *'Plots of Key Results for Beam Section ….'*) three groups of plots. The plot on the left shows the geometry of the selected beam section. The three plots in the middle show the results of both the analytical and the slice method for the Trajectory displacement effect, the Boersch effect and the Space charge defocus obtained respectively. The plot to the right indicates how these effects are – as evaluated by the slice method - built-up over the beam section. You may want to use the *'Previous section'* and *'Next section'* buttons on the top left-hand side of the worksheet to investigate other beam sections from the optical system defined in the worksheet *'System'*. Press the *'Expand all areas'* button in the top left of the worksheet and scroll through the remainder of the sections, which are briefly described in the table below:

Worksheet *'Section'* section title:	Functionality:
Plots of Key Results for Beam Section …	Beam section geometry plot, charts to compare the results obtained with the analytical and slice method and a slice-method generated chart depicting the built-up of the Coulomb interaction effects in the beam section
Plot Parameters & Key Results	User control area to set plot parameters of the charts in the top section and a listing of the key results shown in the middle charts
Beam section … Input Parameters	Input parameters used for the calculation of the Coulomb interaction effects in the beam section
Calculated Theoretical Parameters	Derived theoretical parameters as used in the ETP model, see ref. R-1, R-2 or R-3.
Calculated interaction Effects	Full list of results obtained with the analytical method and the slice method
I and V curves Calculation and Plots	Facility to evaluate the Coulomb interaction effects in the beam section for a range of beam currents and beam potentials
Output tables	Listing of the results obtained for the '*I and V Curves*'

3 INTERAC development environment

3.1 INTERAC program overview

3.1.1 Worksheets overview

The INTERAC workbook consists of 16 user worksheets, which can - in the regular display mode - be selected through the worksheet tabs on the bottom of the screen or – in full screen mode – through the controls on the top of the screen. This table below describes the main function of each worksheet. A more detailed overview is given in the next section.

Worksheet:	Main Function:
Dashboard	Central area from which most program functions are controlled
System	interactive environment to enter, review and modify all system quantities and to specify the model parameters for the different calculation methods. The system plot in the top-section shows the beam optical components, beam geometry, principal rays based on the data shown in the sections below. Various section are included to specify the MC method and the analytical/slice method parameters.
Section	interactive environment to analyze the results of the analytical and slice method for an individual beam section.
MC_in	Input data from the DAT and SYS files for the selected run
MC_out	Output data from the OUT file for the selected run and comparison with the analytical/slice method results.
MC_edi	Output data on the energy distribution from the EDI file for the selected run
MC_sdi	Output data on the spatial distribution from the SDI file for the selected run
MC_pos	Output data on the particle positions from the POS file for the selected run
MC_cor	Output data on the particle co-ordinates from the COR file for the selected run
PlotDis	Plots of the energy and spatial distribution for the selected run
PlotPos	Plots of the final particle positions in the reference plane(s) for the selected run
PlotCor	Plots of the final particle co-ordinates in various "position" and "velocity" views
Runs	Specification of runs in terms of input and output files identifiers
Results	Summary of key input and output data of the MC, analytical and slice method for all runs
PlotRuns1	User specified plots of the selected results from the worksheet *'Results'* using a labeled horizontal axis (e.g. to compare results for various non-related MC parameter settings)
PlotRuns2	User specified plots of the selected results from the worksheet *'Results'* using a continuous horizontal axis (e.g. to compare results for different settings of a single MC parameter)
About	Contains documentation and other general program information
Settings	Program settings on e.g. the main model parameters, numerical and physical constants, Excel calculation mode, and array sizes.

3.1.2 Functionality per worksheet

Dashboard
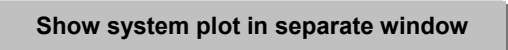
The *'Dashboard'* worksheet groups the key user controls (meaning macro buttons that activate Visual Basic routines) and entry fields to specify the user workspace; to import and export files; to schedule MC batch jobs for background processing; to perform data analysis and calculations; to store results to

memory and to execute spreadsheet management functions (such as the clearance of user data and the reset of the program to its default settings).

System

The *'System'* worksheet provides an interactive environment to enter, review and modify all particle optical system variables and parameters and to specify the model parameters for the different methods. An implicit ray-tracing module displays the beam envelope, the primary rays, the properties of the source, the optical components and the drift, acceleration or deceleration spaces in between the components. The optical properties such as the angular and spatial distributions, optical planes conjugated to the source and the target respectively and corresponding magnifications are estimated by the program to automate the input for the analytical and the slice method.

The program has the capability to advice on or automatically select the optimum MC parameters - such as the sample size and the number of seeds - based on the properties of the beam and certain criteria set by the user, such as the minimum sample length relative to the lateral dimensions of the beam. All parameters can be overwritten by the user if desired.

The system plot and main optical and MC parameters can be shown in a separate window by pressing the macro button *'show system plot in separate window'* (Show system plot in separate window) on the *'System'* worksheet. This function can also be called from some of the other worksheets (e.g. *'Dashboard'*) through the corresponding macro button (Show system). This functionality is provide to obtain a quick snapshot of the essential data derived from the *.sys and *.dat files at any location in the INTERAC workbook.

The analytical and slice method calculations are executed and stored on a per beam section basis. The total system results are derived by adding the results obtained for the different beam sections constituting the total system. Various controls are included to calculate the results for an individual beam section or for all sections in one go. The total system evaluation can be based on the analytical method only, the slice method only or a mix and match of the methods on a per beam section basis, referred to as the "selected results". In the default mode the program automatically selects the best method per beam section and the type of analytical equations used (that is the equations for a beam section with crossover or a parallel beam section). The *'System'* worksheet includes facilities to calculate and plot the analytical/slice method results for various user specified ranges of system input variables in order to analyze the dependency of the system performance on these parameters.

The system data can be stored to file using the formats used by the MC program. The MC program uses two type of input files, the so-called *'system'* file (with extension .SYS) in which the general, mostly "fixed", properties of the source and the optical components are stored and the so-called *'data'* file (with extension '.DAT') in which the "variable" properties such as the beam current and related MC parameters as the sample size and number of seeds are stored. See chapter 4 for further details. No

separate storage is required for the specific input for the analytical and the slice method since all input parameters for these methods are - in the default mode - automatically generated by the program on the basis of the information from the MC SYS and DAT files.

Section

The *'Section'* worksheet provides the means to inspect the results of the analytical and slice method per beam section in more detail. The properties of the individual beam sections can be copied from the *'System'* worksheet. This input can be subsequently modified to analyze the dependency on the model parameters. The analytical and slice method calculations are dynamic, which means that the results are shown immediately after the input has been entered. Ranges of results, denoted as *'user curves'* can be generated to assess the dependency of the Coulomb interactions on the beam current and beam voltage. These curves are calculated be means of control buttons and stored to the output areas on this worksheet. The data is plotted in various graphs. The *'Section'* worksheet is used by the *'System'* worksheet to calculate the interaction effects in the individual beam sections.

MC_in, MC_out, MC_edi, MC_sdi, MC_pos, MC_cor, PlotDis, PlotPos and PlotCor

The data read from the various MC input and output files is stored in the worksheets *MC_in* (*'.DAT'* and *'.SYS'* files containing the system and MC parameters input data), *MC_out* (*'.OUT'* file containing the general output data), *MC_edi* (*'.EDI'* file containing the energy distributions at the target), *MC_sdi* (*'.SDI'* file containing the spatial distributions in the selected reference planes), *MC_pos* (*'.POS'* file containing the lateral particle positions in the selected reference planes) and *MC_cor* (*'.COR'* file containing the complete phase-space co-ordinates of all particles near the target). The energy and spatial distributions are plotted in the worksheet *PlotDis* and the worksheet *PlotPos* and *PlotCor* contain graphs of the positions data and co-ordinates data respectively. These worksheets provide the means to inspect all MC results in full detail and replace the program MCPLOT provided in the previous release of the MonTec package.

The worksheets *MC.pos* and *MC_cor* contain a Macro button (**ShowVectorPlot**) to generate a so-called vector plot showing the displacements from the unperturbed to the perturbed positions. The results are best visible for a limited sample of particles and the user may vary the sample size and "scroll" through the total positions data set by means of the *'next'* and *'previous'* buttons in the bottom section of the vector plot window. When generating the vector plot from the *PlotPos* worksheet, the user has the option to select the perturbed and unperturbed particles positions from different sections of the POS file. Typically, the first section corresponds to the Gaussian image plane of the system and the second section to the plane of best focus. By comparing the unperturbed positions from the first section (Gaussian image plane) to the perturbed positions from the second section (plane of best focus) one obtains the "standard" vector plot, which is – in the default settings - also generated in the *PlotCor* worksheet.

Runs, Results, PlotRuns1 and PlotRuns2

The worksheet *'Runs'* facilitates the file management of all user specified MC runs. The file ID's (that is the file names minus the standard extensions) corresponding to each run are listed on this sheet and associated with a unique run-number. The results of the various MC and analytical calculations are stored in the worksheet *'Results'* using the run-number as the primary key. The worksheets *PlotRuns1* and *PlotRuns2* provide the capability to compare selected results from different runs.

Settings

All key model parameters are aggregated in the worksheet *'Settings'*. The user can modify all settings as desired and simply restore the defaults through the corresponding program controls.

3.1.3 Program conventions

Cell- and font-colors are used systematically to indicate what type of information is displayed; to separate input from output fields and to highlight non-default or invalid input. The main program conventions with respect to cell- and font-colors are the following:

Description:	**Example:**
Worksheet headings:	**About INTERAC**
Worksheet section headings and user instructions:	**Input and Output File Names for Selected Run: 1**
Error messages, warnings or notifications:	**Error reading EDI file: File is empty - No data read.**
Bold numbers are 'hard' input:	**1234**
Normal font numbers represent derived data (that is calculated or linked data):	1234
Yellow boxes with bold numbers denote areas where the user may enter data to specify input:	**1234**
Yellow boxes with normal font numbers denote program generated input data that may be overwritten by the user:	1234
Yellow boxes turn 'signal' red with a white text font when the data entered by the user is invalid (out of range):	**1234**
Yellow boxes turn 'brick' red with a black text font when the data entered by the user deviates from the default setting:	**1234**
Data read from file is shown in light blue area:	1234
Key calculation results are shown in light gray areas:	1234

3.1.4 Display modes

A so-called '*Full Screen Mode'* switch is located in the top bar of each worksheet. It switches the '*Full screen mode'* on and off, with the following effect:

Display mode:	Operation:
Full Screen On	This mode provides the large working-screen display window by removing the standard Excel bars (toolbars, tab sheet bars, etc.) from the bottom and the top of the screen, as well as the slide bar normally on the right side of the screen. INTERAC provides alternative "Sheet Tabs" for the navigation between worksheets on the top of the screen
Full Screen Off	Regular user specified Excel view

The '*System'* and '*Section'* worksheets consist out of various sections (or areas) which can be shown or hidden on an individual basis through the '*Expand'* and '*Collapse'* buttons in the headings of each section. All areas can be expanded or collapsed in one go through the '*Expand all areas'* and '*Collapse all areas'* buttons on the top. Other worksheets have a single '*Expand'* and '*Collapse'* control in the top line to manage the worksheet view.

3.1.5 Worksheet protection

The structure of the workbook as a whole, the individual worksheets and the Visual Basic Code for the various controls are protected to prevent unintended modifications of the code. The graphs can be unlocked for modification by the user through the '*Unlock charts'* controls on the top of the worksheets. The graphs are automatically (re)locked when the user executes an arbitrary control routine.

3.2   INTERAC program functionality

3.2.1 System specification

Go to the worksheet '*System'* and press the macro control '*Set-up screen for system input*' on the right top of the worksheet. You will now see the '*System plot*' on top and below that *the '*Source Properties*'* and '*Optical Components and Drift Sections*' with the corresponding input data. You can reset the input to the Default/Demo system by pressing the macro Control '*Load demo system*'. Alternatively you can create your own system data from a basic data set by pressing the macro control '*Reset for new system*'. The ray-tracing and the corresponding '*System Plot'* creation is performed dynamically, meaning that any changes that you make to the input data are directly reflected in the System Plot (Provided that that the Excel calculation mode is set to '*Automatic*', see worksheet '*Settings*').

To see the effect of changing the data, select the cell in which the focal distance of the condenser lens is specified, which is the entry in the 2nd beam section where at the row with the identifier F. The default entry in the demo system is 0.16 m. You can change the value by typing another value, e.g. 0.12 m. Observe that the change is immediately reflected in the system plot. Another way to change the value in a yellow cell is to select the cell and then press the '*Increase abs',* or '*decrease abs',* '*Increase %' , o*r '*decrease %'* buttons the top-right hand side of the *System* worksheet, which will change the cell entry with the absolute step value or relative % value, specified next to these buttons. Set the entry back to the value 0.16 m.

3.2.2 MC parameter setting

The section '*Monte Carlo Simulation Parameters*', located below the system input sections, specifies the

key MC model parameters. See chapter 4 for an explanation of these parameters. INTERAC provides the facility to set some of these parameters - the sample size NSAM and number of seeds NSEED in particular - automatically. Make sure that that sign *'Automatic'* in the title bar of the section (*'Monte Carlo Simulation Parameters'*) is switched on to set these parameters automatically. INTERAC also estimates the MC run time corresponding to the selected input data and settings. The chart in this section shows the value of the sample length relative to the beam dimensions throughout the system. INTERAC chooses NSAM and NSEED based on the critical ratios specified on the right side below this chart.

3.2.3 Analytical calculation

The section *'Analytical Model Parameters for Coulomb interaction Effects'* of the *'System'* worksheet (Expand this section if it is collapsed) shows the input data used for the Analytical and Slice calculations of the Coulomb interaction effects in the system. INTERAC derives this data automatically from the system input. See references R-1 and R-2 for further information on these parameters.

The section *'Analytical Results for Coulomb interaction Effects'* of the *'System'* worksheet (Expand this section if it is collapsed) contains the output data from the Analytical and Slice calculations by beam section and for the total system at the target. These calculations are not performed "dynamically", but need to be executed by the user through the macro Controls in the top-bar. To calculate the effects in all beam sections as well as the total effect at the target press the *'Calc. All'* button. If you want to inspect the input and the analytical calculation for an individual beam section in more detail, press the button *'Calculate'* above the data corresponding to that beam section. The input data is then copied to the *'Section'* worksheet where the actual calculations for an individual beam section are executed and the results are copied back to the corresponding column in the *'System'* worksheet. You may then visit the worksheet *'Section'* to have a closer look at the input and output data for the selected beam section. The macro controls *'Next section'* and *'Previous section'* on the top left of the worksheet provide an alternative method to load the different beam sections of the total system into the *'Section'* worksheet.

The section *'Comparison of Analytical Results from Different Methods and by Beam Section'* of the *'System'* worksheet (Expand this section if it is collapsed) shows some charts to compare the results obtained with the Analytical, the Slice method and the *'Selected methods'* for the systems as a whole, as well as the results obtained with the *'Selected methods'* in the individual beam sections.

The section *'Analytical Results for Total Energy Spread'* of the *'System'* worksheet (Expand this section if it is collapsed) gives the total energy spread at the target resulting from the energy spread of the source (which is an system input parameter) and the calculated Boersch effect in the system.

The section *'Analytical Results for Total Probe Size'* of the *'System'* worksheet (Expand this section if it is collapsed) gives the results for the total probe size based on the *'Selected methods'* for the Coulomb interaction effects and the calculated geometrical aberrations.

3.2.4 User curves

The results described so far pertain to a single input system setting. Both the worksheet *'Section'* and the worksheet *'System'* provide the capability to evaluate results for a range of input values:

The worksheet *'Section'* has an area entitled *' I and V Curves Calculation and Plots'* were the results for an individual beam section are shown as function of the beam current and beam potential. Different *'variation modes'* can be selected that specify how these quantities are varied. The beam current can e.g. be varied with a constant brightness by increasing the beam lateral dimensions or by changing the brightness with a constant beam geometry. The results are listed in the section entitled *'Output tables'*.

The *'System'* worksheet contains an area entitled *'User Curves'* that provides the facility to calculate the system performance for a range of input values of selected input variables. Any of system input quantities can here be selected as the input variable. The worksheet has a facilitate to "customize" the plots in this section showing the calculation results. The results are listed in the section entitled *'Output tables'*.

3.2.5 Specification of run files

INTERAC associates all input and output files corresponding to an individual MC run and the corresponding analytical/slice calculations with a unique *run-number*. The user can group a series of runs (e.g. for different beam currents in the same system) by entering the same unique Series ID for all runs in the group. The Series ID mechanism provides the capability to execute certain functions in INTERAC for all runs in the Series ID group through a single command.

Select the worksheet *'Runs'* and specify the selected *'run'* and *'series of runs'* as follows:

- In the column with the heading *'DAT file minus ext. (max 10 char.)'* you should enter the DAT file identifier

- In the column with the heading *'SYS file minus ext. (max 10 char.)'* you should enter the SYS file identifier

- In the column with the heading *'Series ID'* you may enter an arbitrary alpha-numerical string for the runs belonging to a certain series

- You may add any comments in the other columns (*'System parameters', 'MC program parameters', 'Remarks'*) to describe the run settings. These columns are added to facilitate the documentation of the different runs and are not directly used by INTERAC.

Select the worksheet *'DashBoard'* and specify a run number in one of the following ways:

- By typing a number in the box entitled *'Selected run no.'*

- By clicking on the macro command buttons *'Next run in series'* or *'Previous run in series'*

- Select another series of runs by clicking on the macro command buttons *'Next series'* or *'Previous series'.* By Entering "All" in the Series ID cell you can select all defined runs through the macro command buttons *'Next run in series'* or *'Previous run in series'*

- In the table with the heading *'Verify Input and Output File Names for Selected Run: ...'* you now see the input and output file names associated with the selected run

3.2.6 Creating MC input data

Once you have defined the system on the worksheet *'System'* you can create the corresponding MC DAT and SYS input files to execute a MC calculation. Vise versa, if you have a system specified through a MC SYS and a MC DAT file, you can load this data to the *'System'* worksheet by importing these files. These export/import operations are controlled from the worksheet 'Dashboard' in the third section (entitled *'Monte Carlo Simulation …'*) and the fourth section (entitled 'Data Analysis for Selected Run: 1') respectively.

In order to export the MC SYS and DAT files go to third section of the worksheet *'Dashboard'* entitled *'Monte Carlo Simulation …'* and proceed as follows. Make sure that the appropriate check boxes on the left side are checked, to ensure that both the DAT and the SYS file are exported. The data that will be exported to file is listed in the worksheet 'MC_in' in the tables entitled *'MC DAT Input/Output file'* and *'MC SYS Input/Output file'*. You may change the input data as specified in the yellow cells of these tables. If you want to export the data from the worksheet *'Systems'* you should check the corresponding box (*'Copy system data first ?'*) to instruct INTERAC to copy this data to the MC_in export area prior to exporting the data to file. You can also execute this copy function from the *'Systems'* worksheet to the MC_in import/export areas through the macro control *'Copy system data to MC_in'* in the top left of the worksheet *'System'*.

The MC file structure allows the use of so-called repeat value indicators ("-1.E00", see also chapter 4) to take-over the last specified the axial co-ordinate (Z) or last specified beam voltage (BV). In the default program setting (as specified in the table entitled *'MC input file parameters'* in the worksheet *'Settings'*) the program uses repeat indicators if specified in the *MC_in* worksheet. You can change the default setting to always store the actual values for Z and BV entries by changing the corresponding setting.

3.2.7 Scheduling and execution of MC batch jobs

Select the worksheet *'Dashboard'.* In the section entitled 'Monte Carlo Simulation ….' you can use various macro functions to either directly run the MC simulation for the selected run or to add the run to the WORKLD.BAT file for batch processing.

Press the macro *'Run job'* to directly run the MC simulation for the selected MC run. The program will create a *'Command Prompt window'* and start the MC simulation. If the MC run files are installed properly you will now see the MC program screen specifying its operations. The window will

automatically close when the MC program terminates.

You can create and modify the WORKLOAD.BAT file for batch processing through the following macro commands:

- Macro Command *'Clear workld'* to remove all existing jobs from the WORLD.BAT file by deleting all file content.

- Macro command *'Add selected job to workld'* to add the selected run to the WORKLD.BAT file.

- Macro command *'Add selected series to workld'* to add all runs from the selected series of runs to the WORKLD.BAT file.

You can use the macro control *'Edit workload'* to inspect the MC runs appended to the WORKLD.BAT file.

Use the control *'Run workload'* to execute the MC runs specified in the WORKLD.BAT file. If the MC runs files are installed properly you will now see the MC program screen indicating that the first job is executed. When this job is finished the WORKLD command structure will automatically start the next job in line. See the MC program documentation (chapter 4) for further details on the workload mechanism. After all job are finished the command prompt window will disappear.

Clearly, you can *'minimize'* the command window while the MC files are processed in the background so that you can continue to work with INTERAC. You can also continue to modify the WORKLD.BAT file when the MC simulations are being executed in the background, because the MC simulation program will only use the WORKLD.BAT file when it has finished a run. It will then open the WORKLD.BAT file, delete the run from the top and start the next run.

As an alternative to the *'Run workload'* control, you can "manually" create a new command prompt window and execute the WORKLD command. For this operation do as follows:

- Start the command prompt in the run-files directory by using the macro command "C:\" (or alternatively: start the *'command Prompt'* under windows and go to the *'MC run file directory'* with the MC.EXE and run-files)

- Enter "WORKLD" at the command prompt and press enter

The only difference with using the *'Run workload'* control is that the command prompt will not vanish after all jobs from the workload are finished.

3.2.8 Importing data for a single run

Select the worksheet *'Dashboard'.* In the table with the heading *'Data Analysis for Selected Run …'* click on one or more of the following macro buttons:

- *'Import MC data and system input files'* to import the input files and write the data to the worksheet

*'MC_in'. W*hen the check box *'Copy input data to system ?'* is checked, the imported data is also copied to the worksheet *'Systems'* and also perform the analytical and slice calculation for the imported system*.*

- *'Import MC OUTfile'* to import the general output file, filter the key data and write the results to the worksheet *'MC_out'.*

- *'Import MC EDI file'* to import the energy distribution output file, write the data to the worksheet 'MC_edi' and set-up the plots in the worksheet *'PlotDis'.*

- *'Import MC SDI file'* to import the spatial distribution output file, write the data to the worksheet 'MC_sdi' and set-up the plots in the worksheet *'PlotDis'.*

- *'Import MC POS file'* to import the positions output file, write the data to the worksheet 'MC_pos' and set-up the plots in the worksheet *'PlotPos'.*

- *'Import MC COR file'* to import the co-oridnates output file, write the data to the worksheet 'MC_cor' and set-up the plots in the worksheet *'PlotCor'*

- *'Import checked files'* to successively execute all previous macro commands for those files that are 'checked' in the boxes to the left

- *'Clear all data'* to clear all data from the worksheets *MC_in, MC_out, MC_edi, MC_sdi, MC_pos, MC_cor.*

You can now inspect the data in the worksheet *MC_in, MC_out* (which lists both the MC results and the analytical / slice method results)*, MC_edi, MC_sdi, MC_pos,* and *MC_cor* and the corresponding plots in the worksheets *PlotDis, PlotPos* and *PlotCor.* Each of the individual charts in the worksheets *PlotDis, PlotPos* and *PlotCor* can be scaled individually (Press the *'Expand'* macro if the scaling data is not visible), but similar plots can be set to the same scale through the *'Same scale similar plots'* macro control.

The worksheet *PlotCor* displays the particles co-ordinates x,y,z,v_x,v_y,v_z in the vicinity of the target through the following set of charts:

- Charts 1-6 (first two rows of charts): Show the lateral x, y and v_x,v_y co-ordinates as function of the axial z-co-ordinates to display the distribution of the particles (accumulated in all samples) in the x,y,x,v_x,v_y,v_z phase space. The red dots refer to the perturbed particle co-ordinates and the blue dots to the unperturbed particle co-ordinates. You can shift the location of the particle co-ordinates along their final velocity by specifying a axial shift distance (*'Zshift'*) in the table on the top of the worksheet and pressing the *'Recalculate plot data'* macro control next.

- Charts 7-9 (third row of charts): The first two charts show the lateral x, y positions of the unperturbed co-ordinates (blue dots) in the reference plane and the lateral x, y positions of the

perturbed co-ordinates (red dots) in the plane of best focus respectively. These positions are calculated by projecting each particle along a straight line determined by its velocity to the relevant plane perpendicular to the axis. The z-co-ordinates of the reference plane and the plane of best focus (Z-co-ordinate of plane of best focus = z-co-ordinate of reference plane z-co-ordinate + defocus distance) are listed in the table on the top of the worksheet. The space charge magnification M is, in the default setting, taken into account by de-magnifying the unperturbed positions with this value. The selection of the reference plane and the handling of the space charge magnification is controlled by the parameters listed in the worksheet *'Settings'* (Section with the title *'Co-ordinates plots parameters'*). The third plot displays the lateral position displacements calculated by subtracting the unperturbed positions in the reference plane from perturbed positions in the plane of best focus. You can redraw the charts for other values for the reference plane (*'Zref'*) , axial defocus distance (*'Δz'*) and magnification (*'M'*) by changing the entries in the table on the top of the worksheet and pressing the *'Recalculate plot data'* macro control next.

- Charts 10-12 (fourth row of charts): Show the histograms corresponding to the lateral positions shown in the charts 7-9 (third row of charts). Through the entry in the table on the top of the worksheet you can choose a histogram corresponding to the distribution of particles in the (radial) R -direction, the X- or the Y-direction (*'Radial dimension parameter'*).

- Charts 13-15 (fifth row of charts): The first tow charts show the lateral v_x and v_y velocities of the unperturbed and the perturbed co-ordinates respectively, similar to the lateral positions plots of charts 7 and 8. The last charts shows the corresponding lateral velocity displacement, similar to the lateral position displacements shown in chart 9.

- Charts 16-18 (sixth row of charts): Show the histograms corresponding to the lateral velocities shown in the charts 13-15 (fifth row of charts). Through the entry in the table on the top of the worksheet you can choose a histogram corresponding to the distribution of particles in the (radial) V_r -direction, the V_x- or the V_y-direction (*'Radial dimension parameter'*).

- Charts 19-21 (seventh row of charts): The first two charts show lateral velocity versus lateral position of the unperturbed and the perturbed co-ordinates respectively. The last chart shows the lateral velocity displacement versus the lateral velocity displacement. The calculation of these phase space diagrams is controlled through the parameters in the table on the top of the worksheet. The parameters affecting the calculation of the lateral positions and velocities are described above. The parameter *'Phase diagram: 1 Absolute values, 2 Positive and negative values'* pertains to these plots in particula*r.*

In addition to the plots which are always displayed in the *PlotPos* and *PlotCor* worksheets one can generate vector plots, showing the displacements from the unperturbed to the perturbed position for each particle, by pressing the *'ShowVectorPlot'* macro control on these sheets, as was outlined in section 3.1.2.

3.2.9 Storing data from all runs

Select the worksheet *'Dashboard'.* In the table with the heading *'Data Storage to Worksheet 'Results''*. Click on one or more of the following macro buttons:

- *'Store data for selected run'* to import the (SYS and DAT) input files, to import and read the general (OUT) output file and/or execute the analytical calculation. The check boxes on the left of this section determine whether INTERAC reads the MC output data file, execute the analytical calculation or does both. The key input and output data for the selected run is written to the worksheets *'MC_out*' and '*Results'.* This function is equivalent to the execution of both the *'Import MC data and system input files'* and *'Import MC out file'* macro commands for the selected run.

- *'Store data for selected series'* to import the (SYS and DAT) input files and the general (OUT) output file, execute the analytical calculation and write the key input and output data for all runs in the selected series to the worksheet *'Results'*. This function is equivalent to the execution of the *'Import MC data and system input files'* and *'Import MC OUT file'* macro commands for all runs in the selected series.

- *'Clear all data from memory'* to clear all stored data from the worksheet.

Go to the worksheet *'Results'* if you want to verify the outcome of this operations.

3.2.10 Plotting results from various runs

Select the worksheet *'PlotRuns1'* (for labeled data - such as the run number - on the horizontal axis) or *PlotRuns2'* (for continuous data - such as the beam current at the target - on the horizontal axis) to plot the data from the worksheet *'Results'*.

In the table *'Select Runs and Specify Line Style & Marker Size'* you can specify a number of sets of runs for which you can want to plot the results. Select the set you want to plot by entering the corresponding number and click on the macro button *'Activate selected set, line & markers'*. Alternatively, you can press the macro controls *'Next set'* or *'Previous set'* to select and activate the next or previous set respectively through a single mouse click. Notice that in the *'PlotRuns2'* worksheet, the selection of the horizontal axis can be specified for each set separately through the cell just below the *'Set 1'. 'Set 2'*, etc. cells. You may change the appearance of the plots by changing the Line style or Marker size through the corresponding entries and by pressing the *'Select Runs and Specify Line Style & Marker Size'* control again next.

In the tables in the section *'Specify Plot Data'* you can specify the quantities to be plotted on the horizontal axis (X-axis) and vertical axis (Y-axis) of the different charts by selecting the corresponding row identifier from the worksheet *'Results'* (The blue column in this worksheet. Expand the worksheet when the blue column is not visible).

You can adjust the scales by specifying the plot range and the type of axis (Linear or logarithmic) in

the corresponding yellow boxes and clicking on the *'Apply scaling'* macro button. By pressing the *'Unlock charts'* button in the top of the worksheet you can select the individual objects of each chart and use any of the regular MS Excel functions to change the presentation of the charts.

3.3 INTERAC file sizes, file names and system structure constraints

INTERAC follows the syntax of the MC program, but has certain restrictions on the number system commands that can be processed and the size of the arrays, as specified in the tables below:

Type of file	Extension	Assumptions
MC-data input file	DAT	Regular syntax as defined in MonTec manual on MC program (chapter 4)
MC-system input file	SYS	Maximum of 10 (DRIFT) sections recorded for system plot (Worksheet ''), each with a maximum of 1 aperture, 1 lens, 1 quadrupole and 1 deflector per section in any combination (optical components are located at the start of the section).
		Two calls to TBR: First call without refocus, 2nd with refocus
		Two calls to RNDTBR/RECTBR: First call without refocus, 2nd with refocus
		Two calls to SYMEBR/ASYEBR: First call before PROCCO, 2nd after PROCCO
		The aperture shape index ISHP=1 for a round or 2 for a rectangular aperture and may not be negative (as in the MC program to represent a so-called "inverted" aperture)
MC- coordinates input/output file	COR	Regular syntax generated by MC program
MC- general output file	OUT	Regular syntax generated by MC program
MC-energy distribution output file	EDI	Maximum of 3 sections: Maximum of 3 calls to SYMEBR / ASYEBR in.SYS file
MC-spatial distribution output file	SDI	Maximum of 4 sections of which at maximum 2 are two-dimensional: Maximum of 4 calls to TBR/RNDTBR/RECTBR and maximum of 2 calls to RECTBR in SYS file
MC- radial positions output file	POS	Maximum of 3 sections: Maximum of 3 calls to STOREP in *.SYS file

Type of array	MC parameter	Assumptions on maximum used
Maximum total number of particles	NTOT = NSEED x NSAM (at target)	60,000
Maximum number of divisions in distribution histograms	NDE,NDT1, NDT2	1,000

4 Monte Carlo simulation program

4.1 General Information

4.1.1 MC program purpose

The program MC provided with the MonTec Particle Optics Simulation Tools package is a Monte Carlo program to simulate electron (or ion) Gaussian beam, shaped beam and projection lithography systems, electron (or ion) scanning microscopes and similar devices. Its purpose is to evaluate the properties of the beam by computing the trajectories of a representative bunch of particles with randomly chosen initial condition. The program takes both the Coulomb interactions between the particles (space charge and statistical effects) and the aberrations of the optical components into account. The optical components are modeled in thin-lens approximation. Dedicated routines are incorporated in the simulation program to analyze the coordinates of the particles at the target plane of the system. The particle positions as well as their energy and spatial distribution can be plotted by means of the INTERAC program, as outlined in chapters 2 and 3.

4.1.2 Manual context

The perspective chosen in this chapter is that of a stand-alone operation of the MC program. Some of this material is less relevant when running the MC program in conjunction with INTERAC, since INTERAC effectively acts as a shell around the MC program. In this mode of operation, many tasks that should otherwise be performed by the user - such as the creation of the input files, the selection of proper values for the various modeling parameters as the sample size and number of seeds and the scheduling of jobs to run on the background through the workload mechanism - are taken care off by INTERAC automatically.

For users running the MC program through INTERAC, this chapter serves to obtain a basic understanding of the MC program in general and the MC system commands and MC model parameters used by INTERAC in particular. Those users may skip the sections covering the hardware and software requirements (section 4.1.5), instructions how to get started when running MC as stand-alone application (section 4.3), instructions how to run the MC program (section 4.4.11), as well as the material on the MC source code organization and compilation aspects (sections 4.48, 4.5.4 and 4.5.5). These sections are, however, relevant for those who run MC as a stand-alone application.

4.1.3 Theoretical basis of the MC program

For a discussion of the Monte Carlo approach in general as well as the physical principles underlying the MC program, the reader is referred to reference R-1 (see section 1.2).

This chapter focuses on the actual implementation of the MC program and the specifics of its operation. The reader is advised to read this chapter in conjunction with the more general description given by reference R-1, chapter 13.

4.1.4 MC program features

The following list indicates the main features of the MC program:

- The executable modules included with the package run on the Windows WIN95, WIN98, WIN2000 or XP operating systems. The use of standard FORTRAN 77 allows straightforward implementation on other computer systems. The MC program has been made operational on various IBM mainframes as well as different types of UNIX systems.

- A dedicated command structure is utilized for a flexible specification of the properties of the simulated beam and column, as well as the required data analysis.

- An extensive set of routines is available to model various types of sources, lenses, quadrupoles, deflectors and apertures.

- A FAST Monte Carlo ray-tracing routine, that utilizes the analytical equations for pair interactions, can be used force as an alternative to the numerical ray-tracing routine with variable time step to compute the trajectories of the particles interacting through the Coulomb. See references R-3 or R-1 for further details on this approach. This FAST ray-tracing routine is one to two orders of magnitude faster than its numerical counterpart without introducing any significant inaccuracies in the final results for practical operating conditions. The two ray-tracing routines are fully compatible and the user can easily switch from one algorithm to another. A third ray-tracing routine is included to model the high current density region of the beam in the vicinity of the source. It introduces so-called *'field'* particles, representing the beam, that interact with the sample of *'test'* particles. The field particles due exert Coulomb forces on the test particles in the sample, but are not perturbed themselves by Coulomb interactions.

- All ray-tracing routines are set up to take a uniform axial electrostatic (accelerating or retarding) field into account.

- Various routines are available to analyze the final coordinates of the particles and to express this data in terms of the total generated energy spread (Boersch effect), the trajectory displacement effect and the space charge defocusing. Special routines are available to evaluate the properties of both Gaussian and shaped spots.

- Facilities are included to compensate finite-size effects (edge effects, due to the finite size of the sample) by means of an axial- position dependent velocity correction.

- The magnitude of various simulation errors, like ray-tracing errors, statistical errors and finite-size errors are indicated.

- A number of Monte Carlo simulations can be run in succession without user intervention (Workload structure).

4.1.5 Hardware and software requirements

The main part of the program package consists of the executable module of the Monte Carlo simulation program MC.EXE. The programs run on a standard PC with a Windows WIN95, WIN98, WIN2000 or XP operating system. The MC program requires less than 1 MB of hard disk space for the executable, but the input / output files can be large depending on the number of particles in the simulation and whether all particle positions and/or co-ordinates are stored as output (*.POS and *.COR files). The dynamic memory requirement depends on the settings of the MONTEC.INC file for the maximum

number of particles in the sample (MSAM) and the maximum total number of particles at the target (MTOT). For MSAM MTOT = 750,000 the program requires about 350 MB DRAM. The programs are written in FORTRAN 77. The programs are compiled and linked with Microsoft FORTRAN PowerStation, version 4.0.

All general source code parameters of the MC program (specifying array-sizes, output units and output formats) are contained in the include file MONTEC.INC. These parameters should be adjusted when recompiling the program for other than Windows based computers. In general, the source code is organized such that all non- standard FORTRAN statements and PC specific output can easily be deactivated in order to comply with different machine configurations. See section 4.5.4 for further details.

4.2 MC program overview

4.2.1 Introduction

Monte Carlo simulation of charged particle beams is a numerical technique in which the trajectories of a bunch of particles, with randomly chosen initial conditions, are traced through a user defined particle optical column. The key-functions of any Monte Carlo program of this type are:

- Generation of the initial coordinates of a bunch of particles.

- Ray-tracing of the particles taking their Coulomb interaction into account.

- Deflection of the particles to represent the optical elements of the column.

- Analysis of the final coordinates of the particles.

The particular realization of the Monte Carlo approach chosen for the MC program is outlined in this section. The purpose of this section is to introduce the reader to the basic concepts of the MC program and its architecture. More detailed information on the functionality of the MC program can be found in sections 4.4 and 4.5. The reader is advised to read this chapter in conjunction with reference R-1, chapter 13.

4.2.2 Command structure

The simulated column is specified by the user by creating a so- called '*MC-system file*' by means of a normal ASCII text editor or by using the INTERAC program. This file contains a series of commands which can be carried out by the program. Various commands are available to represent different types of sources, thin optical components (such as lenses, deflectors, quadrupoles, and apertures), drift spaces and uniform acceleration zones. Other commands instruct the program to process the final data and compute the characteristic properties of the beam, such as its energy distribution, its width (Gaussian beams) or edge-width (shaped beams) in the plane of best focus and the total defocusing caused by the space charge effect. Most commands require the specification of one or more parameters, which should be entered in the so-called parameter fields following the command. Each command and associated command-parameters occupy one or more lines (records) of the MC-system file.

Another input file, called '*MC-data file*', contains the variable beam properties (such as the beam current, voltage and initial energy spread) as well as a number of general program parameters. This set-up makes it easy to run a specific system (defined by the MC-system file) for various operating conditions (defined by different MC-data files). The MC-system file and the MC-data file may contain any number of comment-lines (indicated with a "C" or a "*" in the first column) which are ignored by the program.

4.2.3 Sources and optical elements

The first command in the MC-system file should specify a source, which can be single or a multiple emitter source, specified by the commands SOURCE and MULSRC respectively. The total emission current and acceleration voltage of the source are specified in the MC-data file. The other properties, specified in the MC-system file, concern the (spatial) current density distribution and the initial velocity distribution of the particles at emission. For a single emitter, the current density distribution can be circular with uniform or Gaussian radial distribution or rectangular with uniform distribution. The initial velocity distribution is either specified in terms of the angular distribution (which can be circular uniform or Gaussian) and the energy distribution (uniform, Gaussian or Lorentzian) or in terms of the temperature of the cathode surface, assuming a half Maxwell-Boltzmann distribution (thermionic source). The multiple emitter consists of a rectangular array of emitters of the same type. The type specification is the same as for a single emitter. Both SOURCE and MULSRC utilize a pseudo-random generator to assign a position and velocity to every particle in such a way that their distribution in phase space resembles the specified macroscopic properties. Alternatively, one can specify a test source (with the command TSTSRC) which produces a deterministic distribution of positions and velocities. The test source can be helpful to investigate the optical properties of the column.

The column is modeled as a succession of drift spaces and uniform acceleration zones, separated by thin optical components. The command LENS represents a thin lens, characterized by its focal distance and four aberration coefficients. In addition to the coefficients of spherical and chromatic aberration, one can specify two coefficients representing the rotational errors of a magnetic lens. They pertain to the rotational distortion and chromatic error of rotation respectively. The command DEFLCT represents a deflector, characterized by the deflection angles in x and y direction and a dispersion coefficient. The command QUADRP represents a quadrupole, characterized by its focal distances and chromatic aberration constants in x and y direction, as well as four independent coefficients covering the third order aberrations. The command APERTR should be used to model an aperture, which can be round or rectangular. The aperture can be "inverted" in the sense that it transmits the particles which would normally be stopped and stops the particles which would normally be transmitted. This function is, however, not supported by INTERAC.

In order to account for the misalignment of the column components all optical elements can be shifted with respect to the optical axis. The program permits two or more optical elements at the same axial position, superimposing the action of these elements. In general, the user may specify an arbitrary large number of optical elements. However, the number of apertures should not exceed 20. (as specified by the parameter MAPERT in the file MONTEC.INC), while the number of drift sections should not exceed 100 (as specified by the parameter MDRIFT in the file MONTEC.INC). The representation in INTERAC is, however, limited to a maximum of 10 drift sections and 10 apertures, as specified in

section 3.3.

4.2.4 Ray-tracing routines

The ray-tracing routines calculate the trajectories of the particles in the drift spaces between the optical elements, taking the mutual Coulomb interaction of the particles into account. Different types of routines are available to perform the ray-tracing, represented by the commands DRIFT1, DRIFT2 and DRIFT3. DRIFT1 is based on a numerical ray-tracing algorithm, operating with variable time step. This algorithm provides a straightforward numerical solution of the many body problem. The accuracy of the final coordinates of the particles is limited by the error of the integration process only. The time steps are chosen such that the local integration error does not exceed some user controlled predefined value. The CPU-time required for the numerical ray-tracing increases with the square of the number of particles in the sample and is directly proportional to the number of time steps. CPU- time constraints limit the number of particles in the sample to a maximum of the order 10^5, given current (2003) PC computation speeds. This imposes an upper limit to the beam current that can be simulated at a certain beam voltage.

DRIFT2 is a semi-analytical ray-tracing routine, based on a reduction of the full N-body problem to two-particle interactions. This algorithm is typically one to two orders of magnitude faster than DRIFT1 due to its ability to determine the final coordinates (at the end of the drift section) from the initial coordinates (at the start of the drift section) in a single time step. This approach is therefore referred to as Fast Monte Carlo (FMC) simulation. The reduction to two-particle dynamics is justified as long as most interactions are weak. FMC was found to be extremely accurate for the operating conditions encountered in practical columns, see reference R-3. As far as CPU-time constraints are concerned, the maximum number of particles in the sample which can be handled with FMC is of the order 10^6 with the current (2003) PC computation speeds. However, memory space limitations may impose a somewhat lower limit, as will be indicated later on in this section.

DRIFT3, which is also based on a reduction to two-particle interactions, is intended for the simulation of the high particle density region found in the vicinity of the source. It keeps track of a limited number of sample particles which interact with a large number of field particles, representing the beam. The coordinates of the field particles are not stored to memory. Therefore, the number of field particles can be chosen as large as 10^8.

The ray-tracing routines are fully compatible. For instance, one can simply switch from numerical ray-tracing to analytical ray-tracing by changing the commands in the MC-system file from DRIFT1 to DRIFT2.

All ray-tracing routines permit different beam potentials at the initial and final plane of the "drift" section. The effect of the corresponding uniform electrostatic (accelerating or retarding) field is taken into account. It should be noted that the term "drift" section is used in all cases, whether the particles are accelerated or not.

The interaction between the particles can be switched on or off for each drift section separately. This provides the capability to estimate the individual contributions of the different drift sections to the total effect at the target.

4.2.5 Data analysis

For sample sizes of the order of a few thousand particles or less, it is recommended to employ the facility of the program to repeat the simulation for a number of samples, each starting with a different "seed" of initial conditions. The total number of particles N_{tot} accumulated in all seeds is equal to N_{sam} x N_{seed} , where N_{sam} is the number of particles per sample and N_{seed} the number of seeds. In order to obtain sufficient statistics, N_{tot} should be larger than typically 5.10^3 . The values of N_{sam} and N_{seed} are specified in the MC-data input file. The maximum allowable values for N_{sam} and N_{tot} are determined by the size of the corresponding array, specified by the parameters MSAM and MTOT in the file MONTEC.INC. The PC version of the program MC is compiled with MSAM=750,000 and MTOT=750,000.

The program performs the ray-tracing twice for each sample, one time with the interaction switched off in all drift sections and one time with the interaction switched on or off conform the user specifications given in the MC-system file. When all seeds are carried out, the program has two sets of final coordinates (that is positions and velocities), represented by 2 x 6 x N_{tot} double precision real numbers. Several routines are available to express this information in terms of a few characteristic properties of the beam.

The final energy broadening can be analyzed by using the commands SYMEBR or ASYEBR, for a symmetrical and a (possibly) asymmetrical energy distribution respectively. These routines compute the mean energy, the root mean square (rms) and the Full Width at Half Maximum (FWHM) energy spread, as well as the smallest energy widths containing 10%, 30%, 50%, 70% and 90% of the particles, denoted as FW_{10} , FW_{30} , FW_{50} (or Full Width median), FW_{70} , FW_{90} respectively. A histogram of the energy distribution is formed according to the specifications of the user (given in the MC-data file). The program utilizes a dedicated polynomial fit algorithm to obtain a smooth explicit representation of the energy histogram. The FWHM energy spread is determined from this fit.

The transverse broadening can be analyzed by using the commands TBR, RNDTBR or RECTBR. TBR activates a general routine which evaluates the displacements from the unperturbed trajectories by comparing the coordinates obtained with and without interaction. RNDTBR and RECTBR consider the perturbed coordinates only and apply to a round (Gaussian) and rectangular (shaped) spot respectively. All routines have a facility to seek the plane of best focus, which is usually located somewhat ahead of the Gaussian image plane due to the defocusing action of the space charge effect. A histogram of the spatial distribution is formed according to the specifications of the user (given in the MC-data file). Various width measures are evaluated similar to those mentioned for the energy distribution. The routine activated by the RECTBR command also evaluates the d_{1288} and d_{2575} edge-width of the spot in x and y direction. These measures are essential to characterize the performance of shaped beam systems.

4.2.6 Data storage and plot facilities

The program produces at least one and at most five output files, the exact number depending on the commands specified in the MC-system file. The one file always produced is a general data output file (with default extension .OUT), which contains all general program messages and the main results of the calculations performed by the various routines. The command STOREC issues the storage of the final perturbed and unperturbed coordinates (positions and velocities in double precision real numbers)

to the coordinate file (with default extension .COR). This file can be read by the program during a next run, using the READC command in the MC-system file. The STOREC and READC commands make it possible to re-perform the data analysis without repeating the ray-tracing. The commands SYMEBR and ASYEBR store the data for the histogram of the energy distribution and the corresponding fit to a separate file (with default extension .EDI). The commands TBR, RNDTBR and RECTBR store the data for the histogram of the corresponding spatial distributions and fits to another file (with default extension .SDI). Finally, the command STOREP projects the final positions to a plane perpendicular to the optical axis (with an axial location specified by the user) and stores this data to the positions file (with default extension .POS).

The particle positions (.POS file), energy distribution (.EDI file) and spatial distribution (.SDI file) can be plotted by means of the INTERAC program, described in chapters 2 and 3.

In order to reduce the size of the files for the storage of the coordinates (.COR) and positions (.POS), the program allows for unformatted data storage. The default setting (formatted / unformatted) is determined by the parameters IFORMC (for the coordinates file) and IFORMP (for the positions file), which are specified in the file MONTEC.INC. The PC-version included with this package is compiled with IFORMC=1 and IFORMP=1. This means that the default setting is formatted IO for both the coordinates and the positions. The default setting can be overruled during the interactive file allocation procedure.

4.2.7 Accuracy limitations

The accuracy of a MC simulation is limited by *model errors , ray- tracing errors , statistical errors* and so-called *finite size errors* , see section 4.5.1 or reference R-1, chapter 13, for a detailed description. Special precautions have been made to reduce these errors as much as possible and to estimate their magnitude within the program.

DRIFT1 keeps track of the total integration error in the positions, velocities and energies of the particles caused by the numerical ray-tracing procedure. The nominal number of time steps per meter (set by the parameter NSTEP in the MC-data file) should be taken large enough to rule out this error compared to the statistical error and the finite size errors. DRIFT2 and DRIFT3 keep track of the average number of strong collisions per particle experienced during the flight to indicate the validity of the analytical ray-tracing procedure.

SYMEBR, ASYEBR and TBR estimate the statistical error in the given rms and FW_{50} values by evaluating the spread in the results obtained for a number of sub-ensembles selected from the total set of final coordinates. The statistical error can also be estimated by running the program for different start values of the random number generator (set by the parameter NRAND in the MC-data file).

Finite size errors can in some case be reduced by means of the PROCCO command, which processes the final co-ordinates to compensate for the artificial acceleration experienced by the particles at the edge of the sample, due to the unbalanced space charge force acting on these particles. It evaluates the correlation between the axial velocities and axial position of the particles and adjusts the axial velocities to remove this correlation. PROCCO operates on the final coordinates. A similar procedure can be performed on the intermediate coordinates obtained during the ray-tracing by setting the parameter NPROC in the MC-data input file to 1.

Disregarding model errors, the accuracy of the final results obtained for the FW_{50} values of the energy and trajectory displacement distribution and the (space charge) defocusing distance Δz is estimated to be better than 10% for normal operating conditions. The accuracy of the given FWHM values is in general somewhat worse, due to the fit procedure involved and the critical dependency on the estimate of the central height of the distribution. The accuracy of the predictions for the edge-width values of a shaped spot depends strongly on the number of particles constituting the edge. In general, one requires a substantially larger total number of particles N_{tot} to obtain an accurate prediction of the edge-width than for the prediction of the FW_{50} or FWHM of a central distribution.

4.3 Getting started when operating MC as a stand-alone application

4.3.1 Program files

The following files from the MonTec Particle Optics Simulation Tools package are required for the operation of the MC program:

Executable modules:

MC.EXE   Executable module of the Monte Carlo simulation program. The version delivered with the package runs on an PC with a Windows WIN95, WIN98, WIN2000 or XP operating system.

FORMP.EXE   FORMP.EXE Executable module of the auxiliary program FORMP which is used to transform an unformatted particle positions file (*.POS) to a formatted file which can be read by INTERAC.

MAKEIOF.COM   Executable module of the auxiliary program MAKEIOF which is employed when using the RUN command. It creates the file IOFILES.DAT which contains the filenames of the Input/Output files in the order that they are required by the MC program.

DELINE.COM   Executable module of the auxiliary program DELINE, which is employed when using the WORKLD command structure. It removes the first line of an ASCII file specified as a parameter.

Batch files:

RUN.BAT   Batch file to connect Input/Output files to the MC program, using the default extensions. It utilizes MAKEIOF to generate the file IOFILES.DAT, which specifies the Input/Output filenames to the MC program by means of the DOS feature redirection of IO

WORKLD.BAT   Batch file to run a number of MC simulations in succession without user intervention. It utilizes RUN and DELINE.

Data files:

DEMO1. SYS   Demonstration system input file which is discussed in section 4.4.9.

DEMO1.DAT   Demonstration MC-data input file which is discussed in section 4.4.10.

MC source code files (not included in standard MonTec package):

*.FOR   The MC FORTRAN source code consists of 30 separate files, which are described in section 4.4.8.

MONTEC.INC   Include file which contains the part of the FORTRAN source code where a number of general program parameters are specified. Prior to the compilation and link step these parameters were chosen such to generate an executable module which satisfies the hardware conditions of an PC system (in particular with respect to the available memory space).

4.3.2 Installation

Create a directory on your fixed disk (which is here assumed to be your C disk) and copy the following files delivered with the MonTec package:

- MC.EXE

- MAKEIOF.COM

- DELINE.COM

- RUN.BAT

- DEMO1.SYS

- DEMO1.DAT

Operation limitations

The size of the executable module produced by compilation and linking depends on the array-size specifications given in the file MONTEC.INC. The version of MC.EXE delivered with the package is compiled with the following parameter setting

```
PARAMETER(MSAM=750000,MTOT=750000)
PARAMETER(MDIS=100,MPOL=10,MAPERT=20,MDRIFT=100)
```

The parameters MSAM and MTOT specify the maximum number of particles per sample and the maximum number of particles accumulated in all seeds respectively. See section 4.5.4 for further details.

4.3.3 Running the demo

In order to verify the correct functioning of the MC program, it will here be indicated how to start the demonstration example included in the MonTec package. More details on the demonstration example can be found in sections 4.4.9 to 4.4.11.

Start the Monte Carlo program by entering MC at a command (or DOS) prompt (entering MC means: type "MC" and press). The program will successively ask for:

- a MC-datA (input) file (enter DEMO1.DAT)

- A system (input) file (enter DEMO1.SYS)

- A (input/output) file for the particle coordinates (enter DEMO1.COR)

- A filename for the general output (press for the default name DEMO1.OUT)

- A filename for the storage of the energy distribution (press for the default name DEMO1.EDI)

- A filename for the storage of the spatial distribution (press for the default name DEMO1.SDI)

- A filename for the output of the particle positions (press for the default name DEMO1.POS).

Notice that the program automatically composes a default name for each file by taking the filename of the last specified file and adjusting the extension. After specification of all files the MC status screen appears, which shows a program header, the names of the used MC-data and MC-system file, the time the program was started and the current activity of the program.

An alternative way to start the same demonstration example is to use the RUN batch command (at a command prompt):

    RUN MC DEMO1 DEMO1

The MC program will be started with DEMO1.DAT as MC-data file and DEMO1.SYS as MC-system file. For the other files it uses the names DEMO1+extension (extension: ".COR", ".OUT", ".EDI", ".SDI" and ".POS").

The general results of the simulation are stored in the file DEMO1.OUT. A listing of this file is included in APPENDIX A for comparison. The file DEMO1.POS contains the particle positions in the vicinity of the target plane. The final energy distribution and spatial distribution are stored in the files DEMO1.EDI and DEMO1.SDI respectively. For the interpretation of the output data, the reader is referred to section 4.4.11.

4.4 MC program functionality

4.4.1 Introduction

The user has to specify the input data for the MC simulation by creating two files, namely a MC-data file and a MC-system file. The major part of this chapter is concerned with a detailed description of the formats of the MC-data file (section 4.4.4) and the command language structure on which the MC-system file data definition is based (section 4.4.5). The program produces various output files depending on the commands contained in the MC-system file. The chapter starts with an overview of all input and output files (section 4.4.2). The file allocation procedure is described next (section 4.4.3).

4.4.2 Overview of input/output files

The MC program requires at least two input files and produces at most five output files. The coordinates file (*.COR) can be used both for input and output, depending on the users instructions. In the following, a brief description is given of all types of files used by the MC program.

Input files:

MC-data file (*.DAT)	ASCII file which contains the variable beam properties and general program parameters.
MC-system file (*.SYS)	ASCII file which contains a list of commands (*.SYS) specifying the components of the optical column (such as the source, lenses, apertures and drift spaces) as well as the required analysis of the final coordinates.

Input / Output file:

Coordinates file (*.COR)	ASCII or unformatted FORTRAN file for the IO of the final perturbed and unperturbed coordinates of the particles. The default format is specified by the parameter IFORMC in the file MONTEC.INC (IFORMC=0 for unformatted IO and IFORMC=1 for formatted IO). The default value of IFORMC can be overruled during file allocation. The coordinate file serves as output file when the STOREC command is included in the MC-system file. It serves as input file when the READC command is included.

Output files:

General output file (*.OUT)	ASCII file which contains all general program messages and the main results of the simulation.
Energy distribution (*.EDI)	ASCII file which contains the histogram(s) of the file final energy distribution and the corresponding least square fit(s). The energy histogram is evaluated and stored when the SYMEBR or ASYEBR command is included in the MC-system file. Each of these commands can be issued more than once leading to a series of histograms stored to the same file.
Spatial distribution (*.SDI)	ASCII file which contains the histogram(s) of the file spatial (current density) distribution of the beam and the corresponding least square fit(s). This histogram is evaluated and stored when the TBR, RNDTBR or RECTBR command is included in the MC-system file. Each of these commands can be issued more than once leading to a series of histograms stored to the same file.
Positions file (*.POS)	ASCII or unformatted FORTRAN file for the storage (*.POS) of the final particle positions (perturbed and unperturbed) projected to a plane perpendicular to the optical axis. The plane is specified in the MC-system file as parameter of the STOREP command. STOREP can be issued more than once. The default format is specified by the parameter IFORMP in the file MONTEC.INC (IFORMP=0 for unformatted IO and IFORMP=1 for formatted IO). The default value of IFORMP can be overruled during file allocation.

4.4.3 File allocation

The subroutine PCFILE connects the external input and output files to different FORTRAN units, which are identified by a unit number. The read and write statements of the program source code address the external files by means of this unit number. The choice of unit numbers for the different files is specified by the source code include file MONTEC.INC. See section 4.5.4 for further details.

The input and output filenames can be specified in interactive mode or in batch job mode. In the interactive mode the user starts the MC program and successively answers all requests for file specification. In batch job mode, the file specification is performed by a single command at the (DOS) command prompt, using either the RUN or the WORKLD batch file. RUN is intended to start a single MC simulation. A series of simulations can be started by means of the WORKLD command. These alternatives will now be outlined in more detail.

interactive file specification

Type "MC" at the Command prompt and press . The main program calls the subroutine PCFILE, which directs a request for filename specification to the screen. For each request, the user has the following options:

- Enter the filename of your choice (that is type the filename and press <enter>).

- Press <enter> to use the default filename given by the program.

- Enter "SKIP" (or "skip") when you do not want to connect a file. Clearly, this option should only be used when the corresponding output file is (according to the commands specified in the system input file) not required by the program .

Note: The PC version of the MC program delivered with this package converts all lower case letters of the entered filename to upper case letters. When recompiling the program this convention can be adapted by changing the parameter ICAPT in the source code include file MONTEC.INC (See section 4.5.4 for further details).

File specification by means of the RUN command

The RUN batch file serves to specify all filenames within a single command at the (DOS) command prompt level. The basic form of the command (to be entered at the command prompt) is:

> RUN MC $fname_d$ $fname_s$

where

> $fname_d$ = name of the MC-data input file without extension.

> $fname_s$ = name of the MC-system input file without extension.

For the output filenames the program uses $fname_d$ + the appropriate extension (.COR, .OUT, .EDI, .SDI and .POS).

File specification by means of the WORKLD command

The WORKLD batch file serves to start a series of simulations with different input and output files. Use your own ASCII text editor to change the contents of the file WORKLD.BAT, or use the facilities provided by INTERAC. The simulations to be performed successively should be specified by a series of RUN commands, one command per line (record), entered at the top of the WORKLD.BAT file. For each RUN commands one should use one of the following formats:

RUN MC fname$_d$ fname$_s$ WORKLD

or

RUN MC fname$_d$ fname$_s$ WORKLD fname$_c$

or

RUN MC fname$_d$ fname$_s$ WORKLD fname$_c$ fname$_o$

where

fname$_d$ = name of the MC-data input file without extension.

fname$_s$ = name of the system input file without extension.

fname$_c$ = (optional) name of the coordinates input/output file without extension. The default is fname$_d$.

fname$_o$ = (optional) filename without extension for output files. The default is fname$_d$.

The parameter WORKLD should be included to instruct the RUN batch file to return command to WORKLD after termination of the MC simulation. At first sight, the WORKLD/RUN structure may appear to be somewhat mysterious. However, when using it one will rapidly discover that it provides a convenient and effective method to execute a series of MC runs without the need of user interventions.

The operation of the RUN command can best be understood by studying the contents of RUN.BAT, which is listed below.

```
----------------------------------------------------------------------
ECHO OFF
IF NOT EXIST %2.DAT GOTO END1
IF NOT EXIST %3.SYS GOTO END1
MAKEIOF %2 %3 %5 %6
%1<IOFILES.DAT
:END1
IF NOT EXIST %4.BAT GOTO END2
DELINE %4.BAT
%4
:END2
----------------------------------------------------------------------
```

The user is assumed to be familiar with the operation of DOS batch files and its conventions. The first two lines after the ECHO OFF command verify whether the specified MC-data input file (fname$_d$ -->%2) and system input file (fname$_s$ -->%3) really exist. If so it activates the MAKEIOF program to generate the file IOFILES.DAT, which contains the names of the files which have to be connected to the MC program. MAKEIOF uses the parameters fname$_d$, fname$_s$ and (if specified) fname$_c$ and fname$_o$ as input (fname$_d$ -->%2, fname$_s$ -->%3, fname$_c$ -->%5, fname$_o$ -->%6). Next, the MC program is started, using the DOS feature "redirection of IO" to connect the files specified in IOFILES.DAT. The RUN.BAT concludes by removing the first line of the file WORKLD.BAT (WORKLD-->%4) and returns

control to WORKLD. WORKLD now carries out the command found on the first line, which is the next job in line. This process continues until all command lines of WORKLD have been removed.

4.4.4 MC-data input file

The MC-data input file specifies a number of beam properties as well as the global program parameters. The file may contain any number of comment lines, which should be indicated by a "C" or a "*" in the first column. Comment lines as well as blank lines are ignored by the program. Lines with a blank in the first column (which are, however, not entirely blank) are assumed to be data lines. Each data line of the MC-data file is divided into 6 data fields of 12 columns, separated by an arbitrary character (for which it is convenient to use "|"). All data lines are mandatory and have to be specified in the prescribed order. The order of the entries in the data fields of a data line is also fixed. The location of the data-entry within a data field is arbitrary.

The following table specifies the location of all variables to be specified in the MC-data file:

```
---------------------------------------------------------------------
column:  1          2          3          4          5          6          7
123456789012345678901234567810123456789012345678901234567820123456789012345
---------------------------------------------------------------------
 | PM         | PQ         |
 | BI         | BV         | FWE        | IDE        | ICONS      |
 | INTER      | NSAM       | NSEED      | NFIELD     | NRAND      |
 | NSTEP      | ISTEPA     | IRLIM      | NINT       | IPROC      |
 | NDE        | NTE        | NEHPE      | IFIXE      | PMAXE      |
 | NDT1       | NTT1       | NEXPT1     | IFIXT1     | PNAXT1     |
 | NDT2       | NTT2       | NEXPT2     | IFIXT2     | PMAXT2     |
 | ISTOREE    | ISTQRET1   | ISTORET2   |
 | IMT1       | IMT2       |
---------------------------------------------------------------------
```

The first letter of each variable name specifies the corresponding variable type. Variables starting with a letter in the range A-H or O-Z are reals. Their numerical value should be entered by means of the FORTRAN F-format, E-format or D-format. Variables starting with a letter in the range I-N are integers and should be entered as such. All physical quantities are assumed to be in SI-units.

4.4.5 MC-data variables specification:

PM   = Particles mass in kg

PQ   = Absolute value of the particle charge in elementary-charge units (PQ= | particle charge | / elementary charge).

BI   = Beam current at emission in A.

BV   = Absolute value of the beam voltage at emission in V

FWE   = Full Width at Half Maximum energy spread of the particles at emission in V.

IDE   = Type of energy distribution at emission:
          1 - Uniform
          2 - Gaussian
          3 - Lorentzian

ICONS   = Energy "conservation" specification for source-routine, optical elements and final energy analysis:
          1 - the energy and energy spread of the particles is coupled to their total velocity. The total velocity of each particle is conserved in lenses, quadrupoles and deflectors.
          2 - the energy of the particles is coupled to their axial component of velocity. The axial velocity of each particle is conserved in lenses, quadrupoles and deflectors.

INTER   Global interaction switch:
        0 - Off: No interaction between particles in any drift section.
        1 - On: interaction on or off conform the specifications of the DRIFT commands in the MC-system file.

        Note: The MC program is organized such that the interaction between the particles in a certain drift section is only taken into account when both the global interaction switch INTER (specified in the MC-data) file and the interaction switch associated with that drift section (specified in the MC-system file) are set on. Remember also that all seeds are performed twice. One time to evaluate the unperturbed final coordinates (interaction off) and one time to evaluate the "perturbed" final coordinates. Clearly, the interaction switches in the MC- data and MC-system file apply to the calculation of the "perturbed" coordinates only.

NSAM   = The number of particles per sample (bunch) at emission. (Range: 1 to MSAM, see MONTEC.INC).

NSEED   = The number of seeds to be performed.

NFIELD = Number of field particles used by DRIFT3.

NRAND   = Start value random number generator. The absolute value of NRAND should be in the range: 0 to 214783647. The sign of NRAND determines the type of random generator used. The random generator described in reference R-1 (Appendix 13.A) is used when NRAND<0. An improved version that minimizes any serial correlations is used for NRAND >0 (preferred setting).

NSTEP   = Nominal average number of steps per meter used by DRIFT1.

ISTEPA = Step size algorithm switch for DRIFT1 (See reference R-1):
          0 - No step size variation. Step size is chosen by the program conform the specification of NSTEP.
          1 - New step size determined after every step from the average absolute value of the second and third order terms in the expansions used to update the positions of the particles. The step size is kept within a range which is chosen by the program and which depends on NSTEP.
          2 - As 1, but without step size limitation

3 - New step size determined after every step from the maximum absolute value of the second and third order terms in the expansions used to update the positions of the particles. The step size is kept within a range which is chosen by the program and which depends on NSTEP.

4 - As 3, but without step size limitation.

IRLIM   =   interaction range limitation switch (See documentation for the parameter NINT):

0 - interaction range limitation off.

1 - interaction range limitation on.

NINT   =   Measure for the nominal number of interactions evaluated per particle per time step: If IRLIM=1, the interaction between two particles is taken into account when their mutual distance is smaller than the interaction range RINT and is ignored otherwise. The interaction range RINT is taken equal to NINT times the linear particle density.

IPROC   =   Finite-size error correction switch:

0 - No velocity correction by DRIFT1 and DRIFT2.

1 - z-dependent velocity correction in DRIFT1 (after every time step) and DRIFT2 (at the end of the ray-tracing).

NDE   =   Number of divisions in the energy distribution histogram.(Range: 2 to MDIS, see MONTEC.INC).

NTE   =   Number of terms in the polynomial fit function used for the energy distribution histogram. (Range: 1 to MPOL, see MONTEC.INC).

NEXPE   Specifies the type of polynomial fit function used for the energy distribution histogram (notation: N=NTE):

=   1 - Normal polynomial: $a_N + a_{N-1} x + a_{N-2} x^2 + ... + a_1 x^{(N-1)}$

0 - Even polynomial: $a_N + a_{N-1} x^2 + a_{N-2} x^4 + ... + a_1 x^{2(N-1)}$

-1 - Odd polynomial: $a_N x + a_{N-1} x^3 + a_{N-2} x^5 + ... + a_1 x^{(2N-1)}$

IFIXE   Specification of constraints forced onto the fit of the energy distribution histogram:

=   0 - No constraints.

1 - Fit-function is fixed to zero in the last division.

2 - Derivative of fit is fixed to zero in the last division.

3 - Combination of constraints 1 and 2.

PMAXE   Specifies the maximum energy displacement (from the mean energy) included in the histogram of the energy distribution:

=   >0 - PMAXE specifies the fraction of the total number of particles to be included in the histogram. (Range: 0.1 to 1.0).

<0 - PMAXE specifies the maximum energy displacement included in the histogram: Maximum energy is } PMAXE } ' HWHM, where HWHM is the Half Width at Half Maximum of the energy distribution. (Range: -0.1 to -10.0).

NDT1, NTT1, NEXPT1, IFIXT1, PMAXT1

Specify the formation of the distribution of trajectory displacements (lateral distances between perturbed and unperturbed final coordinates) and the corresponding fit function. These parameters serve as input for the routine TBR (see MC-system file documentation, sections 4.4.6 and 4.4.7) and are similar to those used to specify the formation of the energy distribution histogram (performed by the routines SYMEBR and ASYEBR). See NDE, NTE, NEXPE, IFIXE and PMAXE respectively for further details.

NDT2, NTT2, NEXPT2, IFIXT2, PMAXT2

Specify the formation of the distribution of the final perturbed lateral coordinates, performed by the routines RNDTBR and RECTBR (see MC-system file documentation, section 4.4.7). The meaning of these parameters differs for RNDTBR and RECTBR:

- For RNDTBR the operation of these parameters is completely similar to NDE, NTE, NEXPE, IFIXE and PMAXE respectively, used for the formation of the energy distribution histogram and corresponding fit function.

- For RECTBR:.

NDT2: >0 NDT2 specifies the number of divisions in the total histogram of the spatial distribution in x and y direction respectively.

         <0 NDT2 specifies the number of divisions in the edge of the histogram of the spatial distribution in x and y direction respectively.

NEXPT2: Settings as for NEXPE. In addition:

  2 - Reduced polynomial: a N + a N-1 x 1/(N-1) + a N-2 x 2/(N-1) + ... + a 1 x

  -2 - Reduced odd polynomial: a N x 1/(2N-1) + a N-1 x 3/(2N-1) + ... + a 1 x

Note: The program shifts the origin of the coordinate system used for the fit of the edge (approximately) to the center of the edge. The expectation is that the edge follows an odd function with respect to this origin.

IFIXT2: Specification of constraints forced onto the fit of the edge of the spatial histogram:

0 - No constraints

1 - Continuous joint of the fit of the spot-edge with the intensity level at the center of the spot.

2 - Fit of the spot-edge is horizontal at the boundary with the central intensity level.

3 - Combination of constraints 1 and 2.

PMAXT2: is not active for RECTBR. The program automatically chooses the range of the spatial histogram from the dimensions of the spot.

STOREE = Energy histogram storage switch:

0 - No storage to file

1 - Storage to file

ISTORET1 = Trajectory displacement histogram storage switch (storage to .SDI file):

0 - No storage to file

1 - Storage to file

ISTORET2   =   Spatial histogram storage switch (storage to .SDI file):

0 - No storage to file

1 - Storage to file

IMT1   specifies the Focusing criterion used by the routine TBR (through its absolute value |IMT1|) as well as the type of algorithm used to separate space charge (SC) effects from trajectory displacement (TD) effect (through the sign of IMT1). The routine TBR seeks to minimise the transverse broadening by varying:

(1) The defocusing distance DZ of the final image

(2) The (de)magnification M of the final image (For IMT1>0 only).

The routine thereby effectively eliminates the first order optical effects of the SC "lens" represented by the defocusing distance DZ and the (de)magnification M. The influence of the magnification M is only relevant for large spot/field sizes as e.g. used in projection lithography systems::

=   >0 - TBR will vary both DZ and M (2-dimensional optimization).

<0 – TBR will vary DZ only (1-dimensional optimization), assuming that M=1.

=   1/-1 - Focusing on the FW 50 (Full Width median) value.

2/-2 - Focusing on the FW 90 value.

3/-3 - Focusing on the FWHM value. The FWHM value is determined from the the least square fit of the trajectory displacement histogram.

IMT2   Specifies the Focusing criterion used by the routines RNDTBR and RECTBR. Its operation differs for the two routines:

- For RNDTBR its operation is similar to IMT1, but only positive values are allowed:

1 -   Focusing on the FW 50 (Full Width median) value.

2 -   Focusing on the FW 90 value.

3 -   - Focusing on the FWHM value. The FWHM value is determined from the the least square fit of the trajectory displacement histogram.

- For RECTBR:

1 -   Focusing on the edge-width calculated as the difference between the spot Half Width values containing 95% and 85% of the particles respectively.

2 -   Focusing on the FW 90 spot-width.

3 -   Focusing on the d 2575 edge-width (distance between the 25% and 75% intensity points). The d 2575 edge-width is determined from the least square fit of the edge

4.4.6 MC-system input file

The MC-system file consists of a series of system-commands specifying the optical properties of the simulated column as well as the required data analysis of the final coordinates. The data organization of the system input file is less stringent than that of the MC-data file. Most system commands optional, can be used more than once, while their order is subject to a few rules only.

The MC-system file may contain any number of comment lines, which should be indicated by a "C" or a "*" in the first column. Comment lines as well as blank lines are ignored by the program. Lines with a blank in the first column (which are, however, not entirely blank) are assumed to be data lines. Each

data line of the MC-system file is divided into 7 fields. The first field, which is 6 columns wide, is reserved for a system command. The other fields, which are 10 columns wide each, contain the system command parameters. The fields are separated by an arbitrary character (for which it is convenient to use "|"). Some system commands require more than 6 system command parameters and therefore occupy more than one data line. The continuation lines are characterized by the absence of a system command in the system command field. All command parameters should be specified in the prescribed order. The location of the data-entry within a data field is arbitrary.

The following table shows the available system commands and associated command parameters:

```
-------------------------------------------------------------------------
column:  1          2          3          4          5          6          7
12345678901234567890123456781012345678901234567890123456782012345678901235
-------------------------------------------------------------------------
C Source-commands:
 |SOURCE|  Z        | XCTR     | YCTR     | IDS      | XHW      | YHW      |
       |  IDA      | AHW      | TCA      |
 |MULSRC|  Z        | XCTR     | YCTR     | IDS      | XHW      | YHW      |
       |  NX       | NY       | CX       | CY       | IDA      | AHW      |
       |  TCA      | FWIR     |
 |TSTSRC|  Z        | XCTR     | YCTR     | XHW      | YHW      | NX       |
       |  NY       | AHW      | NA       | NE       |
C
C Ray-tracing commands:
 |DRIFT1|  Z0       | Z1       | BV0      | BV1      | INTER    | IPS      |
 |DRIFT2|  Z0       | Z1       | BV0      | BV1      | INTER    | IPS      |
 |DRIFT3|  Z0       | Z1       | BV0      | BV1      | INTER    | IPS      |
C or
 |DRIFT3|  Z0       | Z1       | BV0      | BV1      | INTER    | IPS      |
       |  ZCTRF    | XCTRF    | YCTRF    | IDSF     | XHWF     | YHWF     |
       |  IDAF     | AHWFF    | TCAF     | IDEF     | FWEF     |
C
C Optical elements:
 |LENS  |  Z        | XCTR     | YCTR     | F        |
C or with aberrations:
 |LENS  |  Z        | XCTR     | YCTR     | F        |
       |  CS       | CC       | RD       | RC       |
 |QUADRP|  Z        | XCTR     | YCTR     | FX       | FY       |
C or with aberrations:
```

```
-------------------------------------------------------------------------
column:  1         2         3        4         5         6         7
123456789012345678901234567810123456789012345678901234567820123456789012345
-------------------------------------------------------------------------
 |QUADRP| Z        | XCTR     | YCTR    | FX       | FY       |
        | C30      | C03      | C21     | C12      | CCX      | CCY      |
 |DEFLCT| Z        | AX       | AY      | DC       |
 |APERTR| Z        | XCTR     | YCTR    | XHW      | YHW      | ISHP     |
C
C Accumulation of final coordinates from successive seeds:
 |ACCUM |
C Storage or retrieval of final coordinates:
 |STOREC|
 |READC |
C
C Data analysis:
 |PROCCO| IMETH    | NDV      | NTVU    | NTVP     | FRACT    | IPS      |
 |SYMEBR|
 |ASYEBR|
 |TBR   | ZREF     | IFOC     |
 |RNDTBR| ZREF     | IFOC     |
 |RECTBR| ZREF     | IFOC     |
 |FOCUS | ZREF     | IFOC     |
C
C Storage of final positions in some reference plane:
 |STOREP| ZREF     | IFOC     |
C
C Program test and termination routines:
 |TESTCL|
 |STOP  |
------------------------------------------------------------------------- .
```

The first letter of each parameter name specifies the corresponding variable type. Parameters starting with a letter in the range A-H or O-Z are reals. Their numerical value should be entered by means of the FORTRAN F-format, E-format or D-format. Parameters starting with a letter in the range I-N are integers and should be specified as such. All physical quantities should be given in SI-units.

As was mentioned earlier, the data organization of the system input file is not very stringent. However, a few rules should be obeyed. To some extend, these rules depend on the presence of the READC command. When the MC-system file does <u>NOT</u> contain the READC command, the following rules apply:

• A MC-system file should contain at least two system commands:
  1) A source command: SOURCE, MULSRC, or TSTSRC.
  2) The ACCUM command to instruct the program to accumulate the final coordinates determined in

the individual seeds.

- The first system command should specify a source.

- The source command, ACCUM command, STOREC command and TESTCL command may only by used once.

- The number of apertures and the number of drift sections should not exceed the values specified by the parameters MAPERT and MDRIFT (See file MONTEC.INC) respectively. The other commands may be used an arbitrary number of times. - All optical element system commands and ray-tracing system commands should be entered after the source command and before the ACCUM command.

- The data storage system commands (STOREC and STOREP) as well as all data analysis system commands (SYMEBR, ASYEBR, TBR, RNDTBR, RECTBR, PROCCO and TESTCL) should be entered after the ACCUM command.

When the MC-system file does contain the READC command the program will ignore all commands concerning the beam definition, that is the source command, all optical element and drift commands as well as the ACCUM command and TESTCL command. The program proceeds directly with the data analysis commands. Accordingly, the constraints given above with respect to the beam defining commands become irrelevant.

4.4.7 System commands and parameters specification

SOURCE: Random initialization of particle coordinates for a single emitter. Parameters:

Z	=	z-coordinate of the emission plane in m.
XCTR	=	x-coordinate of the center of the source in m
YCTR	=	y-coordinate of the center of the source in m
IDS	=	Type of spatial distribution

        1 - Circular uniform distribution with radius XHW.

        2 - Circular Gaussian distribution with Half Width at Half Maximum (HWHM) radius XHW.

        3 - Rectangular uniform distribution with Half Widths XHW and YHW in x and y direction

XHW	=	Half Width in x-direction in m.
YHW	=	Half Width in y-direction in m.
IDA	=	Type of angular distribution:

        1 - Circular uniform distribution with semi-angle AHW.

        2 - Circular Gaussian distribution with Half Width at Half Maximum (HWHM) angle AHW.

        3 - Velocity distribution according to the half Maxwell-Boltzmann distribution, specified by the cathode temperature TCA. This velocity distribution determines both the initial angular and the initial energy distribution. The energy spread specified by FWE and IDE (defined in the MC-data file) is added to the spread determined by TCA.

AHW	=	Beam semi-angle (applies for IDA=1,2) in Rad.
TCA	=	Temperature of cathode surface in K (applies for IDA=3).

N.B.: The emission current BI, the beam voltage at emission BV, the FWHM energy spread FWE and the type of energy distribution IDE are specified in the MC-data file.

| MULSRC: | Random initialization of particle coordinates for a two- dimensional rectangular array of emitters. Parameters: |

MULSRC: Random initialization of particle coordinates for a two- dimensional rectangular array of emitters.
Parameters:

Z	=	z-coordinate of the emission plane in m.
XCTR	=	x-coordinate of the center of the source array in m.
YCTR	=	y-coordinate of the center of the source array in m.
XHW	=	Half Width of the emitter array in x-direction in m.
YHW	=	Half Width of the emitter array in y-direction in m.
NX	=	Number of emitters in x-direction
NY	=	Number of emitters in y-direction. (total number of emitters in the array is NX*NY).
CX	=	Linear contraction in x-direction.
CY	=	Linear contraction in y-direction. The linear contraction is defined as the ratio of the length of the actual emission area and the available length per source. The Half Widths of the individual sources in x and y direction, XHWS and YHWS, are calculated as: XHWS=CX*XHWM/NX YHWS=CY*YWHM/NY.
IDS	=	Type of spatial distribution of the individual emitters: 1 - Circular uniform distribution with radius XHWS. 2 - Circular Gaussian distribution with Half Width at Half Maximum (HWHM) radius XHWS. 3 - Rectangular uniform distribution with Half Widths XHWS and YHWS in x and y direction.
IDA	=	Type of angular distribution of the individual emitters: 1 - Circular uniform distribution with semi-angle AHW. 2 - Circular Gaussian distribution with Half Width at Half Maximum (HWHM) angle AHW. 3 - Velocity distribution according to the half Maxwell-Boltzmann distribution, specified by the cathode temperature TCA. This velocity distribution determines both the initial angular and the initial energy distribution. The energy spread specified by FWE and IDE (defined in the MC-data file) is added to the spread determined by TCA.
AHW	=	Beam semi-angle for the individual emitters (applies for IDA=1,2) in Rad.
TCA	=	Temperature of cathode surface in K (applies for IDA=3).
FWIR	=	Full Width at Half Maximum spread in the beam current of the individual sources relative to the total beam current. The distribution is assumed to be Gaussian.

N.B.: The total emission current BI (produced by all emitters), the beam voltage at emission BV, the FWHM energy spread FWE and the type of energy distribution IDE are specified in the MC-data file.

TSTSRC: Deterministic initialization of particle coordinates for a two- dimensional rectangular array of point-emitters (Test source). Parameters:

Z	=	z-coordinate of the emission plane in m. (Use -1. for last specified z-coordinate)
XCTR	=	x-coordinate of the center of the source array in m.
YCTR	=	y-coordinate of the center of the source array in m.
XHW	=	Half Width of the emitter array in x-direction in m.
YHW	=	Half Width of the emitter array in y-direction in m.
NX	=	Number of point-emitters in x-direction.
NY	=	Number of point-emitters in y-direction. (total number of emitters in the array is NX*NY).

AHW = Beam semi-angle for the individual emitters in Rad.

NA = Number of angular directions per emitter. The routine produces 1 central ray and NA-1 rays at angle AHW, in azimuthal direction equally spaced over 2π .

NE = Number of different energies per ray. The energy deviations relative to the mean energy are equally spaced over the interval FWE (specified in the MC-data file).

N.B.: The total emission current BI and the beam voltage at emission BV are specified in the MC-data file.

DRIFT1: Numerical ray-tracing.

DRIFT2: Analytical ray-tracing.

DRIFT3: Analytical ray-tracing with field particles.

Parameters of DRIFT1, DRIFT2 and DRIFT3:

Z0 = z-coordinate of entrance plane (start drift section) in m. (Use -1. for last specified z-coordinate).

Z1 = z-coordinate of exit plane (end drift section) in m. (Use -1. for last specified z-coordinate).

BV0 = Beam potential in the entrance plane (Z=Z0). (Use -1. for last specified beam potential or the beam potential specified in the MC-data file when no beam potential was specified so far in the MC-system file).

BV1 = Beam potential in the exit plane (Z=Z1). (Use -1. for last specified beam potential).

INT = interaction / boundary condition switch:

    0 - Off: No interaction between particles

    1 - On, using the following boundary conditions (which differ for DRIFT1, DRIFT2 and DRIFT3):

        DRIFT1:   Particle i interacts with all other particles in the sample as long as $z_0 < z_i < z_1$.

        DRIFT2 & interaction between a pair of particles starts when the foremost particle
        DRIFT3: is located in the entrance plane ($z=z_0$).

    2 - On, using the following boundary conditions (which differ for DRIFT1, DRIFT2 and DRIFT3):

        DRIFT1:   : Particle i interacts with particle j as long as both $z_0 < z_i < z_1$ and $z_0 < z_j < z_1$.

        DRIFT2 & interaction between a pair of particles starts when the last particle is
        DRIFT3: located in the entrance plane ($z=z_0$).

    Notes:

      - INT=2 seems most appropriate when the entrance plane ($z=z_0$) coincides with the emission plane of the source. For other cases use INT=1 to switch interaction on.

      - interaction on (INT=1,2) is overruled when the global interaction switch INTER=0 (specified in the MC-data file).

      - Every seed is run twice. One time with the interaction off and one time with the interaction on/off as specified by the switches INTER and INT.

IPS = Printer status switch:

    0 - Reduced output.

    1 - Maximum output.

DRIFT3:   The additional parameters included in the extended (three lines) DRIFT3 command specify the properties of the field particle source. For the usual (one line) - DRIFT3 command the program takes over the source properties specified by SOURCE or MULSRC for the definition of the field particle source. Most of the additional parameters included in the extended DRIFT3 command are equivalent to those used for the SOURCE command (An F, for <u>F</u>ield particles, has been added to all parameter names). The reader is referred to the documentation of the SOURCE system command for further details on these parameters. Two parameters remain (which are for the SOURCE command specified in the MC-data file):

IDEF   =   Type of energy distribution of field particles at emission:
    1 – Uniform.
    2 – Gaussian.
    3 – Lorentzian.

FWEF   Full Width at Half Maximum energy spread of the field particles at emission in V.

LENS: Simulates a thin lens with aberrations (using the two lines LENS command) or without aberrations (using the one line LENS command). Parameters (See reference R-1) for details on the lens algorithm):

Z   =   z-coordinate of the lens-plane in m. (Use -1. for last specified z-coordinate).

XCTR   =   x-coordinate of the center of the lens in m.

YCTR   =   y-coordinate of the center of the lens in m.

F   =   focal length in m.

CS   Coefficient of spherical aberration in m for an object which is located at (minus) infinity.

CC   Coefficient of chromatic aberration in m for an object which is located at (minus) infinity.

RD   Coefficient of rotational distortion of a magnetic lens in Rad.

RC   Coefficient for the chromatic error in the rotation of a magnetic lens in Rad.

QUADRP: Simulates a thin quadrupole with aberrations (using the two lines QUADRP command) or without aberrations (using the one line QUADRP command). Parameters (See reference R-1) for details on the quadrupole algorithm):

Z   =   z-coordinate of the quadrupole-plane in m. (Use -1. for last specified z-coordinate).

XCTR   =   x-coordinate of the center of the quadrupole in m.

YCTR   =   y-coordinate of the center of the quadrupole in m.

FX   =   focal length in x-direction in m.

FY   =   focal length in y-direction in m.

C30   =   Third order aberration coefficient associated with the term x^3 in m.

C03   =   Third order aberration coefficient associated with the term y^3 in m.

C21   =   Third order aberration coefficient associated with the term x^2y in m.

C12   =   Third order aberration coefficient associated with the term xy^2 in m.

CCX   =   Coefficient of chromatic aberration in x-direction in m.

CCY   =   Coefficient of chromatic aberration in y-direction in m.

N.B.: All aberration coefficients refer to an object plane which is located at (minus) infinity.

DEFLCT: Simulates a thin deflector possibly with dispersion. Parameters:

Z   =   z-coordinate of the deflector-plane in m.

AX   =   Angular deflection in x-direction in Rad.

AY   =   Angular deflection in y-direction in Rad.

DC	=	Dispersion (chromatic aberration) coefficient in Rad.

APERTR: Simulates a round or rectangular aperture or disk (inverted aperture). The APERTR command operates on the perturbed coordinates only, see ACCUM command documentation. Parameters:

Z	=	z-coordinate of the aperture plane in m. (Use -1. for last specified z-coordinate).
XCTR	=	x-coordinate of the center of aperture in m.
YCTR	=	y-coordinate of the center of aperture in m.
XHW	=	Half Width of the aperture in x-direction in m.
YHW	=	Half Width of the aperture in y-direction in m.
ISHP	=	Aperture shape/type specifyer:

       1 - Circular aperture with radius XHW.

       2 - Rectangular aperture with Half Widths XHW and YHW in x and y direction.

       -1 - Circular disk with radius XHW.

       -2 - Rectangular disk with Half Widths XHW and YHW in x and y direction.

ACCUM: Accumulates unperturbed and perturbed particle coordinates evaluated in the individual seeds. It stores the corresponding perturbed and unperturbed coordinates to array-memory. The program performs the "interaction off cycle" of a seed first. ACCUM buffers the resulting unperturbed coordinates. The "interaction on cycle" is performed next. When APERTR commands are active, the resulting number of perturbed particles will be smaller than the number of unperturbed particles (since APERTR acts on the perturbed coordinates only). ACCUM stores the perturbed and unperturbed coordinates of those particles which arrive at the end of the system in the "interaction on cycle".

ACCUM interrupts the program when:

- The maximum number of particles (MTOT, see file MONTEC.INC) is stored. The program skips the remaining seeds and continues with the data analysis of the final coordinates.

- The unperturbed coordinate buffer space is full. ACCUM has the facility to store at most MSAM+MTOT/3 unperturbed coordinates per seed, which might be insufficient in the presence of apertures when MTOT<3 x MSAM. See section 4.5.4 for further details.

STOREC: Stores the final perturbed and unperturbed coordinates (accumulated in all seeds) to file.

READC: Reads the final perturbed and unperturbed coordinates from file. When the READC command is included in the MC-system file, the program ignores all commands defining the beam (source commands, drift commands and optical element commands) and continues with the data analysis of the coordinates which are read from file.

PROCCO: Processes final coordinates to correct finite-size effects (or end effects). The z-dependency of the z-component of the particle velocities (for short: z-velocities) is evaluated and compensated. The method is as follows:

The final z-coordinates are divided into a number of z- intervals. The average z-velocity is determined for each interval which results in a z-velocity versus z-position histogram. The z-dependency of the z-velocities is determined by fitting a polynomial function through the histogram. The fit-function serves to evaluate the deterministic z-velocity deviation of all perturbed particles, which is then compensated.

Parameters:

IMETH	=	Compensation method specifyer:

       1 - z-dependency is evaluated of both perturbed and unperturbed z-velocities. The perturbed z- velocities are adjusted such that the difference between both-dependencies is removed.

2 - z-dependency of perturbed z-velocities is evaluated only. The perturbed z-velocities are adjusted such that the z-dependency is removed.

NDV	=	Number of z-position divisions.
NTVU	=	Number of terms of the polynomial fit function used for the unperturbed coordinates.
NTVP	=	Number of terms of the polynomial fit function used for the perturbed coordinates.
FRACT	=	Fraction of particles used in the fit-procedure. The central fraction of the particles is used. (admitted range 0.1< 1).
IPS	=	Printer status:

    0 - No output

    1 - Output of a limited number of characteristic quantities.

    2 - As 1 + output of least square fit function(s).

    3 - As 2 + output of z-velocity versus z-position histogram and corresponding fit values.

SYMEBR: Evaluates the energy distribution of the final perturbed coordinates. The energy distribution is assumed to be symmetrical with respect to the average energy of the particles.

ASYEBR: Evaluates the energy distribution of the final perturbed coordinates. The energy distribution may possibly be asymmetrical with respect to the average energy of the particles. ASYEBR should be used when the source command (SOURCE or MULSRC) represents a thermionic source (IDA=3).

TBR: Evaluates the distribution of trajectory displacements (lateral displacements from the unperturbed positions) in a reference plane from the final unperturbed and perturbed coordinates.

RNDTBR: Evaluates the distribution of the perturbed final positions in a reference plane. The spatial (current density) distribution in the reference plane is assumed to be circular (round) as in Gaussian beam systems.

RECTBR: Evaluates the distribution of the perturbed final positions in a reference plane. The spatial (current density) distribution in the reference plane is assumed to be rectangular as in shaped beam systems. The edge-width of the spot is evaluated.

Parameters of TBR, RNDTBR and RECTBR:

ZREF	=	z-coordinate of the reference plane in m used when IFOC=0. (Use -1. for last specified z-coordinate).
IFOC	=	Focusing switch:

    0 - No Focusing: Spatial distribution evaluated in the plane Z=ZREF.

    -1 - No Focusing: Spatial distribution evaluated in the plane of best focus which was evaluated previously by TBR, RNDTBR or RECTBR. The plane of best focus determined last is taken over. In case no plane of best focus has been determined so far Z=ZREF is used.

    1 - Focusing as specified by the parameter IMT1 (TBR) or IMT2 (RNDTBR/RECTBR), defined in the MC-data file. The Focusing is an iterative procedure which starts with Z=ZREF.

FOCUS: Provides an alternative algorithm for determining the best focal plane by evaluating the image condition in velocity-position phase-space. Parameters:

ZREF	=	z-coordinate of the reference plane in m used as starting condition for the Focusing routine (Use -1. for last specified z-coordinate).
IFOC	=	Plane of best focus update selection switch:

    0 – Reference plane ZREF is NOT updated (Default setting).

1 - Reference plane ZREF set to z-value determined by FOCUS (which can then be used by TBR, RNDTBR and RECTBR by setting the corresponding input variable ZREF=-1).

STOREP: Stores the final perturbed and unperturbed positions of the particles in a reference plane. Parameters:

ZREF = z-coordinate of the reference plane in m used when IFOC=0. (Use -1. for last specified z-coordinate).

IFOC = Plane of best focus selection switch:

0 - Positions evaluated in the plane Z=ZREF.

-1 - Positions evaluated in the plane of best focus which was evaluated by TBR, RNDTBR or RECTBR. The plane of best focus determined last is taken over. In case no plane of best focus has been determined when the STOREP command is called, it uses Z=ZREF.

1 - Take over Focusing performed by TBR. The STOREP command has to be placed after the TBR command.

2 - Take over Focusing performed by RNDTBR or RECTBR. The STOREP command has to be placed after the RNDTBR/RECTBR command.

TESTCL: Test routine which evaluates the following properties for both the perturbed and the unperturbed final coordinates of all particles:

- Velocity of the center of mass
- Average angular momentum relative to the center of mass
- Average potential energy (Coulomb potential due to presence of neighboring particles in the sample)
  + kinetic energy relative to the center of mass.

This data serves to verify whether the conservation laws for momentum, angular momentum and energy are fulfilled. TESTCL should be called after the ACCUM command. It can not be used in conjunction with the READC command.

STOP: Instructs program to ignore the remaining system commands.

4.4.8 Source code organization of MC program

The FORTRAN source code of the MC program is <u>not</u> included with the standard MonTec package. In case you are interested to purchase the MC source code, please contact Caneval BV (See contact information on page 2).

The FORTRAN source code of the MC program is divided into 34 files, which can be compiled separately and linked afterwards. The file MONTEC.INC contains that part of the source code which is shared by many sub-routines. See chapter 4.5.4 for more detailed information. MONTEC.INC is included into the source code by means of the (non-standard) FORTRAN "INCLUDE" statement.

The division of the source code into separate files reflects the organization of the program in terms of functional units. The table below gives an overview of the file names, the function of the included source code and the hierarchy between the functional units. For further details, the reader is referred to the comment contained within the source code files.

Name:	Called by:	Function:
MAIN.FOR	-	Main program. Calls PCFILE and INDATA one time and SYSTEM NSEED times (NSEED is specified in the MC- data input file).
MONTEC.INC	-	Contains a number of parameters which specify array-sizes, unit-numbers and file formats.
PCFILE.FOR	MAIN	Connects program units to external files.
INDATA.FOR	MAIN	Reads MC-data input file and checks input data. Defines the relevant physical and mathematical parameters and initiates program control parameters.
SYSTEM.FOR	MAIN	Reads system input file and calls the appropriate subroutines to perform the system commands. Stores general messages to the general output file. Directs screen through PCSCR.
PCSCR.FOR	PCFILE	Controls output to the screen.
SOURCE.FOR	SYSTEM	Performs system command SOURCE.
MULSRC.FOR	SYSTEM	Performs system command MULSRC
TSTSRC.FOR	SYSTEM	Performs system command TSTSRC.
RANDOM.FOR	SOURCE, MULSRC	Generates pseudo-random numbers.
DRIFT1.FOR	SYSTEM	Performs system command DRIFT1.
DRIFT2.FOR	SYSTEM	Performs system command DRIFT2.
DRIFT3.FOR	SYSTEM	Performs system command DRIFT3
LENS.FOR	SYSTEM	Performs system command LENS.
QUADRP.FOR	SYSTEM	Performs system command QUADRP.
DEFLCT.FOR	SYSTEM	Performs system command DEFLCT.
APERTR.FOR	SYSTEM	Performs system command APERTR.
ACCUM.FOR	SYSTEM	Performs system command ACCUM.
SYMEBR.FOR	SYSTEM	Performs system command SYMEBR
ASYEBR.FOR	SYSTEM	Performs system command ASYEBR
PROCCO.FOR	SYSTEM	Performs system command PROCCO.
TBR.FOR	SYSTEM	Performs system command TBR
TFW.FOR	TBR	Evaluates the radial distribution of trajectory displacements in a given reference plane and computes one or more measures for the width of this distribution.
RNDTBR.FOR	SYSTEM	Performs system command RNDTBR.
RNDTFW.FOR	RNDTBR	Evaluates the radial distribution of the perturbed coordinates in a given reference plane and computes one or more measures for the width of this distribution.
RECTBR.FOR	SYSTEM	Performs system command RECTBR.
RECTFW.FOR	RECTBR	Evaluates the x and y distribution of the perturbed coordinates in a given reference plane and computes one or more measures for the edge- width of these distributions.
FOCUS.FOR	SYSTEM	Performs system command FOCUS which provides an alternative

Name:	Called by:	Function:
		algorithm for the best focal plane by investigating the image condition in velocity-position phase-space.
MINIM.FOR	TBR, RNDTBR, RECTBR, FOCUS RECTFW	1-dimensional and 2-dimensional minimisation routines.
SORT.FOR	SYMEBR, …, RECTFW	Sorts array elements on size in ascending order.
FIT.FOR	SYMEBR, …, RECTFW	Computes least square fit of histograms using a polynomial function.
WIDTH.FOR	SYMEBR, …, RECTFW	Computes width of a distribution from its least square fit function.
IOPAC.FOR	SYSTEM	Input/Output of perturbed and unperturbed particle coordinates and positions. Performs system commands STOREC, READC and STOREP.
TESTCL.FOR	SYSTEM	Performs system command TESTCL.

4.4.9 Demonstration system input file DEMO1.SYS

The input data contained in the file DEMO1.SYS specifies a electron beam projection lithography system resembling the properties of the SCALPEL Proof of Concept (See reference R-2 for a summary or the original data in S.D. Berger et al.,J. Vac. Sci. Technol. B 9. 1996 (1991) or S.D. Berger et al., Proc. SPIE 2322, 434 (1994). The figure below shows the schematics of such a charged particle projector lithography system.
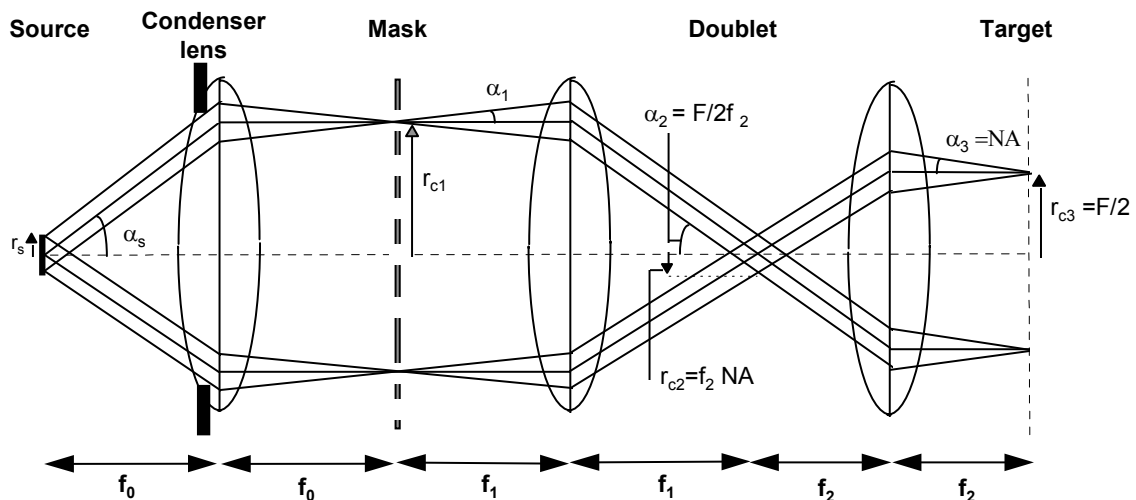
Unlike the conventional electron beam direct write systems, this type of machine uses a relatively wide parallel beam to transfer a mask pattern to the wafer. The illumination system is for the modeling purpose represented by a simple, single condenser lens system. In practice a more sophisticated condenser arrangement may be used to assure a proper uniform illumination of the mask. The mask (also referred to as reticle) is imaged to the target by the lens-doublet with focal distances of f_1 and f_2.

The system can be characterized by the following independent key design parameters: The beam current at the wafer I, beam voltage at the wafer V, system length from mask to target $L_s=2(f_1+f_2)$, magnification from mask to target M, Image field size (edge length of square) F and Numerical Aperture (beam semi-angle at the image plane) NA. The table below lists the default values for these parameters for the DEMO1.SYS system considered here.

System parameter	Symbol	Unit	DEMO1.SYS setting
Beam current at target	I	µA	10
Beam potential	V	kV	100
System length from mask to target	$L_s = 2(f_1+f_2)$	m	0.4
Transverse magnification from mask to target	M	-	0.25
Image field size	F	mm	0.25
Numerical Aperture	NA	mRad	2

This parameter choice implies that $f_0= f_1=160$ mm, $f_2=40$ mm, $\alpha_s=5$ mRad and $r_s=80$ µm, as follows directly from the first order optics of the system. This input data is directly reflected in the DEMO1.YS file, listed below:

```
_____
*************************************************************************
*   MC-SYSTEM INPUT FILE: DEMO1.SYS
*************************************************************************
C
C******     SOURCE, OPTICAL ELEMENTS AND DRIFT SECTIONS :
C
 |SOURCE| 0.000E+00| 0.000E+00| 0.000E+00|        2| 8.000E-05| 8.000E-05|
        |        1| 5.000E-03| 2.500E+03|
 |DRIFT2|   -1.E+00| 1.600E-01|   -1.E+00|   -1.E+00|        0|        1|
 |LENS  |   -1.E+00| 0.000E+00| 0.000E+00| 1.600E-01|
        | 1.600E-01| 8.000E-02| 0.000E+00| 0.000E+00|
 |APERTR|   -1.E+00| 0.000E+00| 0.000E+00| 6.600E-04| 6.600E-04|        2|
 |DRIFT2|   -1.E+00| 3.200E-01|   -1.E+00|   -1.E+00|        0|        1|
 |APERTR|   -1.E+00| 0.000E+00| 0.000E+00| 5.000E-04| 5.000E-04|        2|
 |DRIFT2|   -1.E+00| 4.800E-01|   -1.E+00|   -1.E+00|        1|        1|
 |LENS  |   -1.E+00| 0.000E+00| 0.000E+00| 1.600E-01|
        | 1.600E-01| 8.000E-02| 0.000E+00| 0.000E+00|
 |DRIFT2|   -1.E+00| 6.800E-01|   -1.E+00|   -1.E+00|        1|        1|
 |LENS  |   -1.E+00| 0.000E+00| 0.000E+00| 4.000E-02|
        | 4.000E-02| 2.000E-02| 0.000E+00| 0.000E+00|
 |DRIFT2|   -1.E+00| 7.200E-01|   -1.E+00|   -1.E+00|        1|        1|
```

```
C
C ******     ACCUMULATION AND STORAGE OF FINAL PARTICLE COORDINATES :
C
 |ACCUM |
 |STOREC|
*|READC |
C
C ******     DATA ANALYSIS :
C
 |TBR   |   -1.E+00|          0|
 |RECTBR|   -1.E+00|          0|
 |TBR   |   -1.E+00|          1|
 |RECTBR|   -1.E+00|         -1|
 |SYMEBR|
 |PROCCO|          1|        10|          1|          1| 8.000E-01|          2|
 |SYMEBR|
C
C ******     STORAGE OF PARTICLE POSITIONS IN REFERENCE PLANE(S) :
C
 |STOREP|   -1.E+00|          0|
 |STOREP|   -1.E+00|         -1|
```

_____

The lines with a "C" or a "*" in the first column are ignored by the program. For this file, the following notation convention is used: Lines starting with a "C" are comment lines, while lines starting with a "*" contain temporarily deactivated system-commands. The active lines (starting with a blank) can be analyzed from the description of the system commands given in section 4.4.7. Please, recall that the entries "-1.E+00" refer to default values. For fields specifying an axial location, the default value is equal to the last specified z-coordinate. For fields specifying a beam voltage (present in the DRIFT commands), the default value is equal to the last specified beam voltage or, when beam voltage has been specified so far, it is taken equal to the beam voltage specified in the MC-data input file.

In the remaining part of this section, we will first discuss the optical system specified by DEMO1.SYS and next discuss the system commands pertaining to the data analysis of the final coordinates.

The source specified in the MC-system file represents the virtual source as it is seen from the Condenser lens looking backwards. The modeled source and illumination system represents a simplification from reality, which is adequate because - in a projector system of this type - the mask, rather than the source, is imaged to the target. Hence, the trajectory displacement effect and space charge defocus generated in the beam sections up to the mask do not directly affect the system resolution. This is also the reason for disregarding the interactions in the first two DRIFT sections (The DRIFT command parameter INT=0 in the first two DRIFT commands). The combined energy spread from the source at emission and the Boersch effect generated in the beam up to the mask are accounted for through the input parameter FWE in the MC-DATA file (See section 4.4.10), as well as the parameter IDE specifying the shape of the energy distribution (DEMO1.DAT uses FWE = 1 eV and

IDE=2, implying a Gaussian energy distribution with FWHM = 1 eV).

The total beam consists out of five beam sections (that is five drift spaces). The first two beam sections represent the illumination system. The mask is represented as an aperture at the beginning of the third beam section. The condenser aperture and the "mask" aperture remove about 42% of the total beam current at the source. The beam section following the mask is nearly parallel, followed by the crossover section in between the telecentric lens doublet. The fifth beam section represents the beam in between the second doublet lens and the target.

All specified lenses are assumed to introduce chromatic as well as spherical aberrations. These lens aberrations can simply be switched off by deactivating the second line of each LENS command (which contains the aberration constants), e.g. by placing an asterisk ("*") in the first column of each of these lines.

The data analysis pertains to the spatial distribution (system commands TBR and RECTBR) and the energy distribution (system command SYMEBR) of the beam in the vicinity of the target plane. The target plane is optically conjugated to the mask and the shape of the current density distribution is therefore expected to be square. The most important feature of the spot is its edge-width. The successive commands consider the following properties of the beam:

- TBR (IFOC=0): Distribution of displacements in the Gaussian image plane.

- RECTBR (IFOC=0): Spatial distribution in the Gaussian image plane.

- TBR (IFOC=1): Distribution of displacements in the plane of best focus. This plane is obtained by seeking the axial location for which the width of the distribution of displacements becomes minimum.

- RECTBR (IFOC=-1): Spatial distribution in the plane of best focus. The routine takes over the axial-coordinate determined by TBR (For IFOC=1 it would re-perform the search for the plane of best focus, using its own criterion).

- SYMEBR: Energy distribution. The distribution is assumed to be symmetric, which is consistent with the source specification.

- PROCCO: Performs a correction to the final axial-velocities to reduce finite-size effects. See section 4.4.7 for further details. In general, the user is advised to position the PROCCO command after the TBR, RNDTBR or RECTBR commands, as in the DEMO1.SYS file.

- SYMEBR: Energy distribution after correction of finite-size effects. The results should be compared with those obtained with the first SYMEBR command. The size of the differences indicate the significance of finite size-effects.

The STOREP commands instruct the program to store the positions of the particles in the Gaussian image plane (first STOREP command) and the plane of best focus (second STOREP command) respectively.

4.4.10 Demonstration mc-data input file DEMO1.DAT

The data contained in the file DEMO1.DAT specifies the variable properties of the beam and the general program parameters. The file is listed below:

```
********************************************************************************
*   MC-DATA INPUT FILE: DEMO1.DAT
********************************************************************************
C|          PM|          PQ|
 | 9.10956E-31| 1.00000E+00|
C|          BI|          BV|         FWE|         IDE|       ICONS|
 | 1.00000E-05| 1.00000E+05| 1.00000E+00|           2|           2|
C|       INTER|        NSAM|       NSEED|      NFIELD|       NRAND|
 |           1|        1700|           6|       10000|         123|
C|       NSTEP|      ISTEPA|       IRLIM|        NINT|       IPROC|
 |        2000|           1|           0|        1000|           0|
C|         NDE|         NTE|       NEXPE|       IFIXE|       PMAXE|
 |          50|           6|           0|           0|-2.50000E+00|
C|        NDT1|        NTT1|      NEXPT1|      IFIXT1|      PMAXT1|
 |          50|           6|           0|           0|-2.50000E+00|
C|        NDT2|        NTT2|      NEXPT2|      IFIXT2|      PMAXT2|
*|          40|           6|           0|           0|-2.50000E+00|
 |         100|           6|           1|           3| 9.50000E-01|
C|      ISTOREE|    ISTORET1|    ISTORET2|
 |           1|           1|           1|
C|        IMT1|        IMT2|
 |          -1|           1|
```

As for the MC-system file, the program ignores the lines with a "C" or a "*" in the first column. Lines starting with a "C" are comment lines, while lines starting with a "*" specify an alternative parameter setting. The data specification can be understood from the description given in section 4.4.5. The essential specifications are the following:

- The particles are electrons (as specified by PM and PQ).

- The source emits electrons with an average energy of 100 keV (as specified by BV). The total beam current at the source is 10 μA (as specified by BI). The energy distribution at emission is of the Gaussian type (as specified by IDE) with a FWHM of 1.0 eV (as specified by FWE).

- The simulation consists of 6 seeds (specified by NSEED), each seed starting with a sample of 1700 particles (specified by NSAM).

- The general interaction switch (INTER) is on. No limitation of the interaction range is applied (since IRLIM=0). Finite size effects are not corrected during ray-tracing (since IPROC=0).

- The line specifying the parameters NDT2, NTT2, NEXP2, etc. is selected for the edge-fit performed by RECTBR. The deactivated line (with an asterisk in the first column) applies to RNDTBR.

- All distributions should be stored to file (as specified by ISTOREE, ISTORET1 and ISTORET2).

4.4.11 Running the MC program

It is assumed that you have installed the MC program conform the guidelines given in section 4.3.2. You may start the sample simulation by entering (at a (DOS) command prompt):

RUN MC DEMO1 DEMO1

The simulation takes approximately 12 s on Pentium IV PC with a 1.5 GHz clock speed. After termination of the program, the following output files exist:

- DEMO1.OUT, contains all general messages and results.

- DEMO1.COR. When the STOREC command is included in the MC-system file, this file contains the final coordinates (perturbed and unperturbed) of all particles. The file is formatted and can be examined with a normal (ASCII based) text editor, unless the default setting IFORMC=1 is overruled during the interactive file allocation procedure. The storage of the final particle coordinates to file allows you to re-perform the data analysis without repeating the ray-tracing. The final coordinates can be read from the DEMO1.COR file by activating the READC system command.

- DEMO1.EDI, contains the histogram(s) of the final energy distribution(s), as specified by the SYMEBR commands in the MC-system file.

- DEMO1.SDI, contains the histogram(s) of the final spatial distribution(s), as specified by the TBR and RECTBR commands in the MC-system file.

- DEMO1.POS, contains the final particle positions (perturbed and unperturbed) in the Gaussian image plane and the plane of best focus, as specified by the STOREP commands in the MC-system file.

In the remaining part of this section, the contents of the file DEMO1.OUT will be discussed briefly. The other output files are examined in the next two sections using the plot facilities.

A listing of the file DEMO1.OUT is included in APPENDIX A. Most of the output is self-explanatory. Basicly, the file consists of three parts:

- *Data files and general parameters:* This data is written to the output file by the SYSTEM subroutine during the start of the first seed. It specifies the input files used by the program as well as some general parameters.

- *Specification of system and calculations:* This section contains the messages produced by the source, ray-tracing and optical element routines which are issued by the system commands in the MC-system file. The data is written to file during the last seed (However, error messages of fatal errors are written to file as soon as they occur). A substantial part of the data simply reproduces

the specifications contained in the system and MC-data input file. Some routines, the ray-tracing routines in particular, also produce some numbers which are characteristic for the calculations which have been performed. DRIFT2 gives some statistical information of the two-particle collisions which have been evaluated. The reader is referred chapter 4.5 and reference R.1 for the interpretation of these numbers.

- *Results of Monte Carlo calculation:* This section contains the results of the calculations performed by the various data-analysis routines specified in the MC-system file. Successively, it provides the information obtained by TBR in the Gaussian image plane, RECTBR in the Gaussian image plane, TBR in the plane of best focus, RECTBR in the plane of best focus, SYMEBR before correction of finite-size effects by PROCCO and SYMEBR after this correction. The reader is referred to chapter 4.5 for the interpretation of these numbers.

4.5 Modeling aspects

4.5.1 Accuracy limitations of the mc-program

The accuracy of a MC-simulation is limited by the occurrence of several types of errors. The following error-categories should be distinguished: .

1. Model errors

The representation of the beam and the simulation of optical components within the MC-program relies on a number of simplifying assumptions. All optical components are assumed to be thin and fully described by their first and third order optical properties and chromatic aberration constants. External fields, other than an uniform acceleration field, are assumed to be absent. Stray-fields, mechanical vibrations and electrical charging effects are ignored. Clearly, this list can easily be extended with a number of other obvious simplifications.

Less trivial is the model-error in the formation of the sample in the vicinity of the cathode surface. The particles are randomly distributed over phase-space, reflecting the macroscopic properties of the beam. All correlations between the initial coordinates are ignored in this procedure, which means that some pairs of particles may start with an unrealistically large potential energy. These particles will experience extreme large deviations from their unperturbed trajectories, which may not correspond to reality. For that reason the tails of the resulting energy and trajectory displacement distributions should be viewed with some caution. In general, large displacements should be disregarded in the data-analysis. Distribution width-measures which are insensitive to the exact tails of the distribution (such as the Full Width median value (FW_{50}) and the Full Width at Half Maximum (FWHM)) are therefore preferred above those which are dominated by a few large displacements (such as the root mean square (rms) value).

2. Ray-tracing errors

The numerical ray-tracing (used by DRIFT1) is affected by an integration error, which depends on the size of the time-step Δt. The local integration error, in the positions and velocities, is of the third order in the time step Δt. Therefore, the total integration error is of the second order in Δt. This implies that an increase of the integration accuracy by a factor A, requires a factor $A^{1/2}$ more time steps, leading to

a corresponding increase in CPU-time. The total integration error is estimated by the program and the user can directly verify whether the accuracy of the ray-tracing has been sufficient or not.

The errors generated by the analytical ray-tracing (used in DRIFT2 and DRIFT3) are related to the reduction to pair interactions. Within the two-particle model, the calculation of the displacements can be considered as exact. The reduction to pair interactions is justified as long as the average number of strong interactions per particle, experienced during the flight, is small. This number is counted by the analytical ray-tracing routine and is printed out, which provides an indication of the validity of the Fast Monte Carlo (FMC) approach. In this connection, it should be noted that the errors in the final coordinates, due to the occurrence of strong collisions, are of a stochastic nature, which has favorable effect on the overall accuracy of the FMC approach. Furthermore, it was found that the error in the prediction of the statistical properties of the beam (like the width of the energy and trajectory displacement distribution) is significantly smaller than the error in the exact final coordinates of the individual particles. See reference R-3 for a more detailed discussion on this topic. .

3. Statistical errors

The accuracy of the estimation of the statistical properties of the beam is related to the total number of particles N_{tot} , accumulated in all seeds ($N_{tot} = N_{sam}$ x N_{seed}). The statistical error in the rms-value and the FW_{50} value of the energy and trajectory displacement distribution are estimated within the program, which allows a direct verification by the user. As an additional test, one can run the same simulation a number of times, using different start values for the random number generator (which is specified in the MC-data input file). By observing the variation of the final results, one obtains some idea of the statistical error involved. In order to improve the statistical accuracy by a factor A one has to increase N_{tot} by a factor A^2 . This should be done by running more seeds. Accordingly, the CPU-time, which is directly proportional to the number of seeds, increases with a factor A^2 . .

4. Finite size errors

The qualification "finite-size effect" is used to denote all apparent interaction effects, present in the final results of a MC- simulation, which are related to the inadequate representation of the beam by a sample of particles of finite size. The following finite-size effects are distinguished:

- Underestimation of the interaction effects due to an insufficient sample length L_{sam} . In this case, a particle does not have enough "neighbors" to represents the total beam. In other words, the sample length can not be considered as large compared to some effective interaction range. The effective interaction range depends on the linear particle density and the beam geometry. In addition, it differs for the various interaction phenomena. For instance, the total Boersch effect, generated in a beam segment with a narrow crossover, stems predominantly from the crossover area. For the simulation of this effect in this geometry, it is therefore sufficient to take the sample length L_{sam} an order of magnitude larger than the crossover radius. However, the trajectory displacement effect, generated in the same beam geometry, is not necessarily dominated by the contribution of the crossover area. A significant contribution may stem from the dilute parts of the beam and a proper simulation requires a larger L_{sam} than for the Boersch effect. The space charge effect has even a longer effective interaction range and a proper simulation requires a larger sample than for the statistical effects. The situation is again different for a nearly cylindrical beam

segment, in which all parts of the beam contribute equally to the various interaction phenomena, leading to longer effective interaction distances than for a beam segment with a narrow crossover. Clearly, the particles near the edge of the beam, always experience a deficiency of interacting neighbors. N_{sam} should be large enough to render their contribution insignificant relative to the contribution of the particles which have sufficient neighbors.

- Improper estimation of the interaction effects due to the unbalanced space charge force acting on the particles near the edge of the bunch. It may cause an underestimation as well as an overestimation of the interaction effects. The Boersch effect is, in general, the most strongly affected by this kind of finite-size effect. The particles at the front of the bunch experience an artificial acceleration, while the particles in the back are artificially retarded. Accordingly, the generated axial velocity spread (Boersch effect) is overestimated. However, the unbalanced space charge force also causes an increase of the sample length during the flight, which leads to an artificial reduction of the linear particle density and a corresponding reduction of all interaction effects.

The application of z-dependent velocity correction, on the intermediate coordinates or the final coordinates, leads to some reduction of finite-size effects and provides insight in their magnitude. In general, one should choose the number of particles in the sample N_{sam} large enough to assure that these effects are insignificant. An increase of N_{sam} by a factor A, leads to an increase of the required CPU-time by factor A^2 , assuming that the interaction range of the particles is not limited. .

Conclusions

As far as CPU-time is concerned, one sees that the reduction of finite-size errors and statistical errors both lead to an quadratic increase with a certain accuracy improvement factor A, whereas the integration error of the numerical ray-tracing shows a square-root dependency on A. Therefore, when using numerical ray-tracing, it is a good strategy to choose the nominal number of steps per meter N_{step} large enough to rule out the contribution of integration errors. In order to run the program economically, one should take N_{sam} and N_{seed} such, that the finite size error and the statistical error are of the same magnitude.

Clearly, model errors are more difficult to estimate. The major problems occur with the simulation of the beam in the source area, as can be understood from the preceding analysis. Disregarding model errors, the accuracy, obtained for the defocusing distance and the FW_{50} values of the energy and spatial distribution, is estimated to be better than 10%, for normal operating conditions. The accuracy of the calculated FWHM values, is in general somewhat worse, which is related to the use of the polynomial fit procedure and the reliability of the estimation of the central height of the distribution. The accuracy of the predictions for the edge-width of a shaped spot, depends strongly on the number of particles constituting the edge. In general, an accurate estimation of the edge-width requires a substantially larger number of particles N_{tot} than the estimation of the FW_{50} or FWHM width of a central distribution.

4.5.2 Recommended settings of program parameters

The MC-data input file and the system input file contain a substantial number of parameters which

should be specified by the user. With respect to the run-time of the program and the accuracy of the final results, the following parameters are the most critical: The number of particles per sample N_{sam}, the total number of seeds N_{seed}, the number of field particles N_{field} (when using DRIFT3), the nominal number of integration steps per m N_{step} (when using DRIFT1) and the interaction range NINT (when using interaction range limitation: IRLIM=1). The optimum setting of these parameters depends strongly on the operating conditions, such as the beam geometry and the current density. Accordingly, it is difficult to formulate detailed prescriptions for the setting of these parameters which hold generally. Other parameters, depend less strong on the operating conditions and specific settings are more easy to recommend. This applies in particular to the parameters pertaining to the data analysis. Finally, there are also parameters which are mainly included to give the user some freedom of choice in the operation of the program. No recommended settings are given for these parameters.

We will first give some guidelines for the setting of the parameters for which the best choice depends critically on the operating conditions. Some remarks on the parameter setting for the correction of finite size effects will be given next. The chapter concludes with a general table for the recommended settings of all (non-arbitrary) parameters.

Selecting N_{sam} and N_{seed}

In principle, the criterion for the choice of the number of particles in the sample N_{sam} is simple: It should be large enough to make the finite-size effects negligible and small enough to keep the required CPU time within reasonable limits. However, the errors caused by finite-size effects are hard to predict since they depend strongly on the beam geometry and particle density in the beam and also differ for the various interaction phenomena. The required CPU time is more easy to estimate: It increases with the square of N_{sam} and is directly proportional to the number of seeds N_{seed}. The square dependence of the CPU time on N_{sam} implies that one can usually not afford to choose N_{sam} much larger than strictly necessary. Furthermore, N_{sam} is limited by memory space considerations. Its maximum value is determined by the parameter MSAM (which is specified in the file MONTEC.INC). As finite size effects are hard to predict beforehand, while CPU-time considerations forbid to exceed the critical sample size by a large factor, the choice of a proper N_{sam} is somewhat a trial and error process.

The total number of particles accumulated in all seeds is equal to $N_{tot} = N_{sam} \times N_{seed}$ (where N_{sam} represents the average number of particles per sample at the target, which may be smaller than the number specified at the source due to the presence of apertures in the simulated column). Given a certain $N_{sam} \times N_{seed}$ should be chosen large enough to keep the statistical error in the final results within acceptable limits. Usually, a choice which assures that $N_{tot} > 5.10^3$ leads to acceptable statistics. However, a larger total number of particles is required to obtain a reliable estimate of the edge width of a shaped spot. The maximum value of N_{tot} is limited by memory space considerations and is specified by the parameter M_{tot} (which is specified in the file MONTEC.INC). In the previous chapter it was explained that in order to run the MC program economically, one should select N_{sam} and N_{seed} such that the finite size errors and statistical errors are approximately of the same size.

The MC program evaluates a number of quantities which give some indication of the various error contributions. These quantities may serve to verify the reliability of a simulation without having to repeat the simulation with a different parameter setting. The accuracy of the ray-tracing is estimated by the various drift routines. The routines SYMEBR, ASYEBR and TBR provide measures for the rms

statistical errors in the predicted broadening effects. Finite size effects can partly be corrected by using the PROCCO system command or by setting IPROC=1 in the MC data file.

The PROCCO command is particularly useful to estimate and control finite-size effects. The impact of finite size effects on the Boersch effect can be estimated by instructing the MC program to calculate the energy spread both with and without processing of the final coordinates (By including the SYMEBR or ASYEBR command twice in the MC-system file, one time before the PROCCO command and one time after). It is interesting to study the dependency of the resulting energy spread on the number of particles in the sample N_{sam}. For very small N_{sam}, the energy spread will be underestimated. This can be understood from the fact that the interaction force between the particles in a thin slice is directed perpendicular to the beam axis. With increasing N_{sam} and in absence of correction of the final coordinates, the spread increases to a value which is too large, due to the artificial deceleration and acceleration of the particles near the edges of the bunch. With further increasing N_{sam}, their contribution gradually becomes insignificant and the observed energy spread levels off to the correct value. In presence of correction of the final coordinates, the energy spread is expected to increase monotonically with the number of particles in the sample N_{sam} and reaches the correct value for a smaller sample-size than without correction. By studying the results both with and without correction, one obtains a lower and an upper limit for the correct energy spread at a relative small N_{sam}.

To verify the validity of a MC-simulation with respect to finite size effects, one has to check whether an increase of N_{sam} affects the outcome of the simulation significantly or not. If so, the sample was too small and one has to perform the simulation again with a larger sample. This aspect of running MC-simulations requires a certain experience of the modeller. A clear understanding of the mechanisms involved is indispensable to obtain reliable results, without consuming large amounts of CPU-time.

Let us consider the sample simulation of sections 4.4.9 and 4.4.10, specified by the DEMO1.DAT and the DEMO1.SYS files, as an example. In order to make the dependency on the sample size explicit, one should run the simulation a few times in succession with for instance the following range of values for N_{sam} and N_{seed}:

Run no:	2	3	4	5	6	7	8
N_{sam}:	200	500	1,000	2,000	5,000	10,000	20,000
N_{seed}:	100	40	20	10	4	2	1

Notice that the total number of particles at the source $N_{tot} = N_{sam} \times N_{seed}$ is 20,000 for each run in this series. Due to the presence of the two apertures, about half of the current is removed during the flight through the system. Therefore, at the target N_{tot} is in the order of 10,000 particles. The set of runs specified in the table is included as part of the INTERAC sample sessions (See INTERAC worksheet *'Runs'*, Runs 2 to 8). The results obtained for the Boersch effect, the trajectory displacement effect and space charge defocus for this series of runs are shown in the figures below (Taken over from INTERAC worksheet PlotRuns1).

Boersch effect

TD effect & SC defocus

Legend left: FW50E-BP, FW50E-AP, FW50E-I&S
Legend right: FW50R-BF, FW50R-AF, FW50R-IA, DZF-MC, DZF-IA
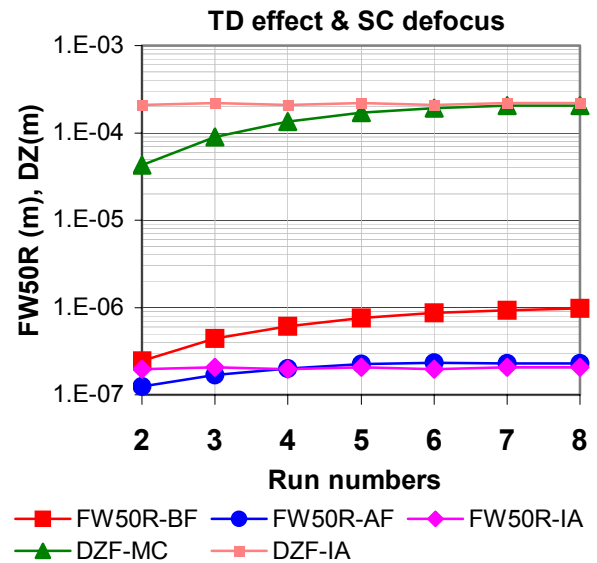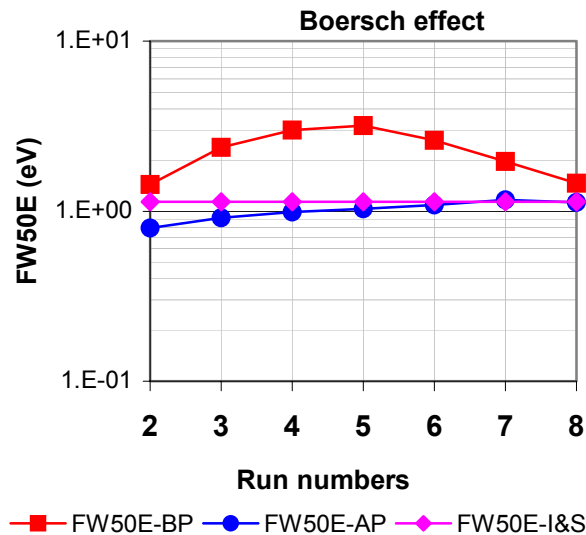
In the left hand side plot, FW50E-BP and FW50-AP represent the FW_{50} energy spread at the target as evaluated by the MC program before running the PROCCO routine and after running the PROCCO routine respectively and FW50E-I&S is the FW_{50} energy spread calculated with the INTERAC analytical equations accounting for both the Boersch effect and the energy spread of the source. In the right hand side plot, the FW50R-BF and FW50R-AF are the FW_{50} spatial broadening as evaluated by the MC program before and after refocusing and FW50R-IA is the trajectory displacement effect calculated with the INTERAC analytical equations. The quantities DZF-MC and DZF-IA in this figure represent the space charge defocus evaluated with the MC program and the INTERAC analytical equations respectively.

When comparing the FW50E-AP with the FW50E-I&S figures in the left hand side plot, one sees that these results converge from approximately run number 5 onwards. This suggests that a sample size of 2000 particles at the source is adequate to make the finite size effects for the Boersch effect sufficiently small, provided that the PROCCO routine is used prior to the evaluation of the final energy spread. When PROCCO is not used, on requires a sample size that is about 10 times larger to ensure that finite size effects are negligible for the Boersch effect. Indeed the value obtained before running PROCCO is always larger that the value obtained after running PROCCO and tends to overestimate the Boersch effect when finite size effects are significant.

When comparing the FW50R-AF with the FW50R-IA figures and the DZF-MC with the DZF-IA figures in the left hand side plot, one sees that these results also converge from approximately run number 5 onwards. Thus a sample size of 2000 particles is (also) sufficiently large to assure that finite size effects are negligible for both the trajectory displacement effect and the space charge effect. Please, bear in mind that these results are particular to the sample system considered here and will in general depend on the beam geometry and the particle density.

A practical method to obtain an estimate for the minimum sample size that is required to render finite size effects insignificant is to compare the sample length to the radial dimensions of the beam. This method is in fact used by INTERAC when it automatically selects the sample size. In the default setting NSAM is chosen such that the sample length is at least 5 times the minimum beam radius and at least 2 times the maximum beam radius in all sections of the beam. The default criteria can be changed by the user if desired (See the section '*Monte Carlo Parameters*' in the worksheet '*System*'). This method

provides adequate results in most cases. However, absolute certainty that finite size effects are negligible indeed can only be obtained by repeating the MC simulation with an increased sample size, as outlined above.

Alternative methods for correction of finite size effects

The PROCCO system command provides a method for reducing finite size effects by processing the final co-ordinates of the particles near the target. Finite-size effects can also be corrected during the ray-tracing performed by the DRIFT1, DRIFT2 and DRIFT3 system commands, by setting the parameter IPROC in the MC-data file to 1. The differences between both correction methods can be summarized as follows:

- PROCCO acts on the final perturbed coordinates of all particles accumulated in all seeds. The compensation applied by the drift routines when IPROC=1 is performed after each time step for each seed separately. As far as the dynamical-aspects of the ray-tracing is concerned, the last method may yield better results in case of strong finite size effects.

- The statistical approach used by PROCCO is more sophisticated than that used by the drift routines for IPROC=1. PROCCO can avoid overcompensation by accounting for the fact that a part of the z-dependency in z-velocities is also present in the unperturbed coordinates. Furthermore, PROCCO is set up to use higher than first order polynomial fit functions. As far as the statistical aspects of the compensation method are concerned PROCCO is preferred.

From these considerations it follows that PROCCO provides the best approach to compensate moderate finite size effects. It is therefore recommended to set IPROC=0. However, in case of strong finite size effects the setting IPROC=1 may improve the accuracy of the final results. The user should be aware that this approach may lead to overcompensation of finite size effects. The user is referred to the general table given below for further details on the PROCCO command parameters.

List of recommended settings

The numbers given in the following table should be interpreted as guidelines not as rules. The parameters which are not included do not directly affect the accuracy of the results, nor the required CPU-time.

1 - MC-Data input file:

Parameter:	Recommended setting:	Remarks:
NSAM	> 100	See previous remarks in this section on finite size effects.
NSEED	NSEED > 5.10^3/NSAM	A total number of particles 5.10^3 provides good enough statistics for most conditions. A higher number of particles is usually required to obtain a reliable estimate of the edge-width of a shaped spot.
NFIELD	>> NSAM, < 10^8	The required CPU time for the ray-tracing of DRIFT3 is directly proportional to NSAM x NFIELD. As far as memory space is concerned, there are no restrictions on NFIELD.
NSTEP	> 1000	Provides sufficiently accurate numerical ray-tracing with DRIFT1 for normal conditions.
ISTEPA	1	Bounded variable time step controlled by the average higher order terms in the position expansion is appropriate unless one is specifically interested in the exact final coordinates of the strongly deflected particles (use then ISTEPA=3 or 4).
IRLIM	0	Use no interaction range limitation within the sample unless a thorough check on the results for different NINT is done.
IPROC	0	Use PROCCO for the correction of finite-size effects.
NDE/NDT1/NDT2	20 - 60	Number of divisions in histogram should be large enough to establish a sufficient resolution and small enough to have a significant number of particles per division.
NTE1/NTT1/NTT2	4 - 6	Number of terms in fit should be large enough to provide enough degrees of freedom to follow the shape of the distribution and small enough to smooth the (statistical) noise.
NEXPE/NEXPT1	0	Use a symmetric function for the fit of energy and displacement distribution.
NEXPT2	0	In combination with RNDTBR.
	-1, 1	In combination with RECTBR.
IFIXE/IFIXT1	0,1,3	Largely a matter of taste.
IFIXT2	0,1,3	In combination with RNDTBR.
	3	In combination with RECTBR
PMAXE/PMAXT1/ PMAXT2	-2.0 - -3.0	Maximum value in distribution should be either 2 to 3 ' HWHM or be set such 0.85 - 1.0 that the distribution contains 85% to 100% of the particles.
IMT1/IMT2	1	Focusing on width-values which are determined from a least square fit should be avoided since this might lead to an excessive long run time.

2 - System input file:

System command:	Parameter:	Recommended setting:	Remarks:
PROCCO	IMETH	1	Removes correlation in axial position and axial velocity generated by particle interactions only.
	NDV	>= 2, <= 10	The number of particles per division should be large.
	NTVU,NTVP	1	Correct for linear dependency only.
	FRACT	>=0.7, <=0.9	Exclude particles on the edge of the sample from the analysis.
TBR / RNDTBR	IFOC	0,1,2	The quality of the Focusing depends on the exact conditions. Focusing RECTBR IFOC 0,2 on the edge-width (RECTBR with IFOC=1) is not recommended.

4.5.3 Interpretation of output data

In this chapter it will briefly be discussed how to interpret the data of the general output file (*.OUT file). For an example of such a file, the reader is referred to Appendix A, which contains a listing of the file DEMO1.OUT.

The general output file consists of three sections. The contents will be discussed per section.

1 - Data files and general parameters

The data contained in this section is self-explanatory. It is stored by the subroutine SYSTEM during the first call by the main program. Verify whether the correct input files have been connected to the program. The start value of the random number generator is a critical overall parameter and is therefore included in the listing. Due to the statistical nature of the results, the exact values of a specific simulation can only be reproduced when using the same start value for the random number routine.

2 - Specification of system and calculations

This section contains the messages of the source, optical elements and ray-tracing routines which are specified in the MC-system file. During the last seed, each routine stores the values of the input parameters. Some routines also give the values of some characteristic parameters which provide insight in the performance of the routine. The statistical quantities represent averages over all seeds (not just the last seed).

Verify whether you have entered the correct values for the various parameters. Most of the characteristic properties produced by the routine are self-explanatory. However, the DRIFT2 and DRIFT3 routines supply statistics which may need some explanation. When the interaction is on (MUTUAL INTERACTION 1 or 2) the routines keep track of the different types of two-particle collisions and the strength of the two-particle interactions. Different equations are employed to evaluate weak

interactions (using first order perturbation dynamics), complete interactions (using nearly complete collision dynamics) and strong incomplete collisions (using full collision dynamics). The routines specify the average number of times each type of calculation is performed per particle per seed (the average is evaluated over all seeds). The reduction to two-particle interactions requires that most interactions are weak. Accordingly, the majority of calculations should be performed by means of first order perturbation dynamics.

To provide another measure for the validity of the reduction to two-particle interactions, the DRIFT2 and DRIFT3 routines keep track of the number of strong collisions (measured in terms of the size of the resulting deviation) per particle experienced during the flight through the drift section. The relative deviation in position and velocity is evaluated for each collision. The program counts the number of collisions which lead to a larger deviation than 0.05, 0.1, 0.15 and 0.5 respectively. Especially the last number should be small compared to unity.

Another indication for the strength of the interactions is given by the average, minimum and maximum value of the eccentricity parameter $q=b/b_\perp$ (in the listing denoted as B/B(90)), where b is the impact parameter and $b_\perp$ the value of the impact parameter which corresponds to a 90 degrees deflection. The validity to two-particle interactions requires that strong deflections are rare, which means that the average value of $b/b_\perp$ should be very large compared to unity.

3 - Results of Monte Carlo calculation

This section contains the messages of all routines that perform the analysis of the final coordinates. These routines are activated after the last seed has been performed. The messages appear in the output list in the same order as the system commands are specified in the MC-system file. Again most data is self-explanatory.

The formation of the energy and spatial histograms and corresponding fits is performed by the program conform the specifications of the user given in the MC data file (parameters NDE, NTE, ... , PMAXT2). Verify (also by investigating the plot-data contained in the *.EDI and *.SDI files) whether the histogram-range, the division width and the quality of the fit are appropriate to obtain reliable FWHM (routines SYMEBR, ASYEBR, TBR and RNDTBR), d_{2575} and d_{1288} (routine RECTBR) width measures. For the spatial distributions, the FWHM, d_{2575} and d_{1288} width measures are evaluated both in x-direction (projection of particle positions to the x-axis) and in y-direction (projection of particle positions to the y-axis). In case of a round or square beam, these numbers should approximately be the same. The deviations between the numbers obtained in x-and y-direction provide some insight in the reliability of the statistics and the fit procedure. The routines TBR and RNDTBR focus on the distribution along the radial coordinate R. It should be noticed that the corresponding FWHM ($FWHM_R$) is in general not identical to the FWHM in x- and y-direction (this is only the case when the distribution is Gaussian).

The routine RECTBR uses an iterative procedure to obtain the best edge-fit. The procedure is carried out separately for the plots in x- and y-direction. It selects a fit-range (with boundaries XW0 and XW1 for the plot in x-direction and boundaries YW0 to YW1 for the plot in y- direction) and an appropriate shifted coordinate system which is centered such that the edge-contour can be described by an odd-function with respect to the origin. The corresponding positional shifts are SHIFTX and SHIFTY in x- and y-direction respectively. The corresponding shifts of the intensity coordinate (distribution height) are

DSHIFTX and DSHIFTY in x- and y-direction respectively.

All routines evaluate a number of different width-measures and leaves the choice of the best characteristic property to the user. As far as accuracy is concerned, one should realize that:

- The distribution width-measures which are evaluated without using a fit-function (rms-values, FW_{10}, FW_{30}, FW_{50}, FW_{70}, FW_{90}) are in general more reliable than those which do rely on the use of a fit-function.

- The tails of the displacement distributions (corresponding large displacements) are the most susceptible to errors. Firstly, since the large displacements are primarily caused by pairs of particles which are initially very close to each other. The generation of such pairs may not correspond to reality. Secondly, large displacements are the most susceptible to ray-tracing errors, which is true both for DRIFT1 (integration error) as for DRIFT2/DRIFT3 (reduction to pair interactions breaks down when a particle experiences two or more strong interactions in the same drift section). Thirdly, as the number of particles in the tails is small, an enormous total number of particles is required to obtain reliable statistics. From these arguments one should conclude that those width measures which depend strongly on the tails of the distribution (such as the rms and FW_{90} values) should be viewed with some caution.

- Width measures which are determined by just a few particles (such as the FW_{10} width) are strongly affected by statistical errors.

From the preceding arguments it follows that the FW_{50} (full width median) is in general the most reliable width measure. However, from the experimental point of view one is often more interested in a FWHM or a d_{1288} value. The best approach is to keep track of these quantities as well as the FW_{50}-value.

When performing a series of simulations, the user is advised to compare the following output quantities:

Routine	Operating condition:	Characteristic output:	Remarks:
SYMEBR/ ASYEBR	before PROCCO	FW_{50} , FWHM	Energy width without correction of finite size effects. after PROCCO idem Energy width with correction of finite size effects.
TBR and RNDTBR	IFOC=0	$FW_{50,R}$, $FWHM_R$, $(FWHM_X + FWHM_Y)/2$	Spatial broadening in Gaussian image plane.
	IFOC=1,2	idem + defocusing Δz	Spatial broadening in plane of best focus and defocusing distance. (IFOC=1 recommended).
RECTBR	IFOC=0	d_{2575}–average, d_{1288}-average	Edge-width in Gaussian image plane
	IFOC=1,2	idem + defocusing Δz	Edge-width in plane of best focus and defocusing distance. (IFOC=2 recommended).

Trends can best be estimated from the FW_{50} of the energy and spatial distributions, the d_{2575} edge-width and the defocusing distance Δz. The FWHM and d_{1288} values are usually most suited for comparison with experiment.

4.5.4 Source code parameters in file MONTEC.INC

This section is only relevant when you have access to the FORTRAN source code of the MC program. The FORTRAN source code of the MC program is <u>not</u> included with the standard MonTec package. In case you are interested to purchase the MC source code, please contact Caneval BV (See contact information on page 2).

The file MONTEC.INC is included (by means of the non-standard FORTRAN INCLUDE statement) in all subroutines except in RANDOM and SORT. It contains a number of global source code parameters, defining array-sizes, input/output (IO) units and some other IO properties. The comment incorporated in MONTEC.INC specifies the detailed functioning of the various parameters.

Specification of array sizes

For the executable module of the MC program delivered with this package the total number of particles (MTOT) was set to 750,000, the maximum number of divisions in the distribution-histograms (MDIS) was set to 5000, the maximum number of terms in the polynomial fit-functions (MPOL) was set to 10 and the maximum number of apertures (MAPERT) and drift sections (MDRIFT) were set to 20 and 100 respectively.

When recompiling the program these sizes can be adjusted by editing the file MONTEC.INC. When changing MTOT and MSAM the following considerations should be kept in mind:

- Some compilers require the size of a labeled common block to be smaller than 64 Kbytes. The sample particle coordinates are stored in the common blocks C1P (positions) and C1V (velocities), see for instance the source code in the file ACCUM.FOR. Each array-element represents a double precision (8 byte) real. The size of these common blocks is therefore equal to 3 x 8 x MSAM. The accumulated particle coordinates are stored in the common blocks C5P (perturbed positions), C5V (perturbed velocities), C6P (unperturbed positions), C6V (unperturbed velocities). The size of these common blocks is equal to 3 x 8 x MTOT. Accordingly, a 64K limit implies that MSAM and MTOT should be smaller than 2666.

- Each seed is performed twice. One time with the interaction switched off (generating the unperturbed coordinates) and one time with the interaction switched on or off according to the user specifications (generating the perturbed coordinates). When apertures are included a part of the perturbed coordinates may possibly be removed from the sample during the ray-tracing through the column. However, this information is not available until the calculation of the perturbed trajectories has been completed. Meanwhile the program has to store the unperturbed coordinates of all particles in the sample. The ACCUM routine stores these coordinates into the arrays PXF0, PYF0, PZF0 (final unperturbed positions), VXF0, VYF0 and VZF0 (final unperturbed velocities). Any excess data is stored into the dummy arrays TEMP1 and TEMP2 of size MTOT. The program can buffer up to MTOT/3 unperturbed particles above the normal MTOT elements stored in the regular

arrays (PXF0, PYF0, ... , VZF0). Accordingly, the program may run out of buffer space (during the last seed) when the fraction F of transmitted particles is smaller than 1-MTOT/3*MSAM. When MTOT>3*MSAM this condition will never occur, but it may occur for smaller values of MTOT. In that case the routine ACCUM will generate an error message.

The following (probably evident) considerations should be kept in mind when changing MDIS, MPOL, MAPERT and MDRIFT:

- The number of divisions in the distribution histogram arrays is set by the parameters NDE (energy distribution) NDT1 and NDT2 (spatial distributions), which are specified in the MC data file. The parameter MDIS should be chosen equal to or larger than the maximum number of divisions required by the user.

- The number of terms in the polynomial fit function is set by the parameters NTE (energy distribution), NT1 and NT2 (spatial distributions), which are specified in the MC data file. The parameter MPOL should be chosen equal to or larger than the maximum number of terms required by the user.

- The maximum number of apertures and drift sections specified in the MC-system file may not exceed MAPERT and MDRIFT respectively.

Specification of Input/Output units and format

The MC program uses seven Input/Output units for the data transfer to and from files. In addition, two units are reserved for the output to the screen and the input from the keyboard respectively. The unit references in the read/write statements of the source code are given in terms of the parameters IUNIT1 to IUNIT9. These parameters are set in the file MONTEC.INC.

The parameter IOMODE can be used to select different IO modes. When IOMODE=0 all output to the screen and the interactive file specification is suppressed. It is assumed that the files are connected to the program units in an external fashion. This mode may be used when running the program on the background on a mainframe type of computer. The setting IOMODE=1 leads to an interactive file specification, but suppresses all PC specific code to address the screen (in particular the so-called DOS escape sequences) as well as any non-standard FORTRAN 77 functions to evaluate the time and date functions. For IOMODE=2, the MC program will call certain (non-standard FORTRAN 77) functions to evaluate the time and date at the start and the finish of the program and calculate the total run-time. For IOMODE=3, the MC program utilizes certain DOS-escape sequences to clear the screen and format the output to the screen. This setting is obsolete when running the program under WIN2000 or XP. The MC program delivered as part of the MonTec package has been compiled with IOMODE=2.

The default format used for the positions (*.POS) and coordinates (*.COR) files are set by the parameters IFORMP and IFORMC respectively. The value 0 corresponds to unformatted IO and the value 1 to formatted IO. Unformatted IO leads to a substantial reduction in file size, but prohibits file editing with a normal ASCII text editor. When using interactive file specification, the default values can be overruled during the file allocation. The MC program delivered as part of the MonTec package has been compiled with IFORMP = IFORMC=1 and therefore creates formatted positions and co-ordinates files, unless this parameter is overruled during the dynamic file allocation.

Some computer system distinguish between lower and upper case letters. With the parameter ICAPT one can select whether the filenames should be converted to lower case letters (ICAPT=1) or upper case letters (ICAPT=2) or should be left as they are entered (ICAPT=0).The MC program delivered as part of the MonTec package has been compiled with ICAPT=2.

The twelve character long string VERSN is printed in the MC status screen and can be used to indicate the program version.

4.5.5 Non-standard FORTRAN and PC specific source code

The MC program contains a limited number of statements which deviate from the FORTRAN 77 standard. Although most compilers will support the types of non-standard FORTRAN statements used, the exact implementation may vary per compiler. When recompiling the program with another compiler than the Microsoft FORTRAN PowerStation (version 4.0), the user should take care of these compiler dependent statements by proper modification.

PC specific source code is used to perform screen operations as "clear screen" and "position cursor" when the IOMODE parameter in the MONTEC.INC file is set to 3. These functions are executed through so-called DOS escape sequences which are written to IUNIT6 (console). For other than PC compatible systems these characters are meaningless and will be displayed on the screen (The same thing happens with DOS when the ANSI.SYS file is not installed properly or when the wrong ANSI.SYS version is used). For PCs running under Windows WIN2000 and XP the use of DOS escape sequences is considered to be obsolete. The MC program delivered as part of the MonTec package has been compiled with IOMODE=2 and does not issue DOS escape sequences.

MC source code

The MC program uses the following non-standard FORTRAN 77 statements:

* The INCLUDE statement is used in the MAIN program and all subroutines except in RANDOM and SORT.

* The functions GETTIM and GETDAT are used in the subroutine PCSCR to obtain the current time and date when the MONTEC.INC parameter IOMODE = 2 or 3. The start time is displayed on the screen. In order to provide information on the runtime of the program, the time and date at the start and the end of the program are both printed at the end of the general output file (*.OUT).

* Backslash editing is used for the output to the screen in the subroutine PCSCR. The backslash ("\") in the output format suppresses the separation of the current record and the next record (in other words, it suppresses a line feed).

All PC specific source code can be suppressed by setting the parameter IOMODE, contained in the file MONTEC.INC, to 0 or 1.

5   References and background information

Further background information on the theoretical basis of the analytical models used for estimating the effect of Coulomb interactions and the Monte Carlo simulation technique can be obtained in the following publications:

- **R-1.** G.H. Jansen, *Coulomb interactions in Particle Beams* (Advances in Electronics and Electron Physics, Suppl. 21,Academic Press, Boston, 1990)

- **R-2.** G.H. Jansen, Journal of Applied Physics, Vol.84, No 8, p. 4549 (1998)

- **R-3.** G.H. Jansen (1987). "Fast Monte Carlo Simulation of Charged Particle Beams", J. Vac. Sci. Technol. B, 5 (1987)

- **R-4.** P.Kruit and G.H. Jansen, *Space Charge and Statistical Coulomb Effects* (Handbook of Particle Optics Handbook, Ed. Jon Orloff, CRC Press, New York 1997)

Reference R-1 provides a full description of the alternative approaches to calculate the impact of Coulomb interactions in particle optical systems. The analytical equations derived in this publication on the basis of the so-called Extended Two Particle approach are used by INTERAC to calculate the Boersch effect, the trajectory displacement as well as the space charge effect. A more condensed version of the theory for Coulomb interactions is presented in reference R-4. Reference R-3 introduces the specifics of the so-called Fast Monte Carlo Simulation technique which is based on a decomposition of the full N-particle ray-tracing algorithm on to two-particle interactions, which is also covered by R-1.

Reference R-2 describes some modification to the extended two-particle model to improve the accuracy of the predictions of the trajectory displacement effect in particle beam projection systems. The theory outlined in reference R-1 was developed for probe forming systems, such as electron and ion scanning microscopes and Gaussian or shaped beam lithography systems. Fit-functions are used within the theory to express part of the numerical output into explicit analytical prescriptions. These functions were found to become inaccurate for the relatively wide beams typically used in the more recently developed projection type lithography systems. New fit-functions are presented in reference R-2 which extend the applicability of the theory to the wide beams and doublet configurations used in projection systems. Reference R-2 also describes some modifications to the Monte Carlo program to account for the first order space charge magnification effect. This effect could be ignored for the relatively small spots of Gaussian and shaped beam systems, but would yield a significant overestimation of the trajectory displacement effect - assumed to be identical to the remaining blur after refocusing - for the wide images used in projection type of systems.

Appendix A.   **MC DEMO1.OUT output file listing**

_____

```
          ************************************************************
          *                                                          *
          *                                                          *
          *        MONTE CARLO SIMULATION OF PARTICLE BEAM SYSTEMS    *
          *                                                          *
          *                    (C) G.H.JANSEN, 1989-2003             *
          *                                                          *
          *                                                          *
          ************************************************************



             ****       DATA FILES  AND GENERAL PARAMETERS       ****


DATA   INPUT FILE ....................................DEMO1.DAT
SYSTEM INPUT FILE ....................................DEMO1.SYS
PARTICLE COORDINATES INPUT/OUTPUT FILE ...............DEMO1.COR
NUMBER OF SEEDS .......................................       6
TYPE OF RANDUM NUMBER GENERATOR .......................       2
START VALUE FOR RANDOM NUMBER GENERATOR ...............     123



             ****    SPECIFICATION OF SYSTEM AND CALCULATIONS    ****


ROUND SOURCE(2) LOCATED AT Z  (IN M) .................. 0.00000D+00
     SOURCE (HWHM) RADIUS (IN M) ...................... 8.00000D-05
     SPATIAL DISTRIBUTION (1=UNIFORM, 2=GAUSSIAN) ......       2
     BEAM SEMI-ANGLE (IN RAD) ......................... 5.00000D-03
     ANGULAR DISTRIBUTION (1=UNIFORM, 2=GAUSSIAN) ......       1
     FULL WIDTH ENERGY SPREAD (IN EV) ................. 1.00000D+00
     ENERGY DISTR. (1=UNIFORM, 2=GAUSSIAN, 3=LORENTZIAN)       2
     PARTICLE MASS (IN KG) ............................ 9.10956D-31
     PARTICLE CHARGE (IN C) ........................... 1.60219D-19
     NUMBER OF PARTICLES IN THE SAMPLE ................     1700
     NOMINAL SAMPLE LENGTH (IN M) ..................... 5.10843D-03
     ACTUAL SAMPLE LENGTH [AVERAGE FOR ALL SEEDS] (IN M) 5.10430D-03
     BEAM VOLTAGE (IN V) .............................. 1.00000D+05
     TOTAL BEAM CURRENT (IN A) ........................ 1.00000D-05
DRIFT2: ANALYTICAL CALCULATION OF TRAJECTORIES
     DRIFT SECTION NUMBER .............................       1
     START DRIFT LENGTH AT Z0 (IN M) .................. 0.00000D+00
     END DRIFT LENGTH AT Z1 (IN M) .................... 1.60000D-01
     BEAM POTENTIAL (IN V) ............................ 1.00000D+05
     TIME OF FLIGHT FROM Z0 TO Z1 (IN S) .............. 8.53093D-10
     MUTUAL INTERACTION (1,2=ON, 0=OFF) ...............       0
THIN LENS(2) AT Z (IN M) ............................. 1.60000D-01
     FOCAL LENGTH (IN M) .............................. 1.60000D-01
     SPHERICAL ABERRATION COEFFICIENT (IN M) .......... 1.60000D-01
     CHROMATIC ABERRATION COEFFICIENT (IN M) .......... 8.00000D-02
     ROTATIONAL DISTORSION COEFFICIENT (IN RAD) ....... 0.00000D+00
     ROTATIONAL CHROMATIC ABERRATION COEFF. (IN RAD) ... 0.00000D+00
RECTANGULAR APERTURE    1 AT Z (IN M) ................ 1.60000D-01
     HALF WIDTH IN X-DIRECTION (IN M) ................. 6.60000D-04
     HALF WIDTH IN Y-DIRECTION (IN M) ................. 6.60000D-04
     AVERAGE NUMBER OF PARTICLES INCIDENT PER SEED .....     1700
```

```
      AVERAGE NUMBER OF PARTICLES THROUGH PER SEED ......    1383
      TOTAL BEAM CURRENT THROUGH (IN A) ................. 8.13529D-06
DRIFT2: ANALYTICAL CALCULATION OF TRAJECTORIES
      DRIFT SECTION NUMBER .............................       2
      START DRIFT LENGTH AT Z0 (IN M) .................. 1.60000D-01
      END DRIFT LENGTH AT Z1 (IN M) .................... 3.20000D-01
      BEAM POTENTIAL (IN V) ............................ 1.00000D+05
      TIME OF FLIGHT FROM Z0 TO Z1 (IN S) .............. 8.53093D-10
      MUTUAL INTERACTION (1,2=ON, 0=OFF) ...............       0
RECTANGULAR APERTURE     2 AT Z (IN M) ................ 3.20000D-01
      HALF WIDTH IN X-DIRECTION (IN M) ................. 5.00000D-04
      HALF WIDTH IN Y-DIRECTION (IN M) ................. 5.00000D-04
      AVERAGE NUMBER OF PARTICLES INCIDENT PER SEED .....    1383
      AVERAGE NUMBER OF PARTICLES THROUGH PER SEED ......     850
      TOTAL BEAM CURRENT THROUGH (IN A) ................. 5.00000D-06
DRIFT2: ANALYTICAL CALCULATION OF TRAJECTORIES
      DRIFT SECTION NUMBER .............................       3
      START DRIFT LENGTH AT Z0 (IN M) .................. 3.20000D-01
      END DRIFT LENGTH AT Z1 (IN M) .................... 4.80000D-01
      BEAM POTENTIAL (IN V) ............................ 1.00000D+05
      TIME OF FLIGHT FROM Z0 TO Z1 (IN S) .............. 8.53093D-10
      MUTUAL INTERACTION (1,2=ON, 0=OFF) ...............       1
      PROCESSING OF END-EFFECTS OF SAMPLE (1=YES,0=NO) ..      0
      INTERACTION RANGE LIMITATION (1=YES,0=NO) ........       0
      AVERAGE NUMBER OF CALCULATIONS USING FIRST ORDER
        PERTURBATION THEORY PER PARTICLE ............... 8.32636D+02
      AVERAGE NUMBER OF CALCULATIONS USING COMPLETE
        COLLISION DYNAMICS  PER PARTICLE ............... 0.00000D+00
      AVERAGE NUMBER OF CALCULATIONS USING FULL
        COLLISION DYNAMICS  PER PARTICLE ............... 1.83638D+01
      AVERAGE NUMBER OF STRONG COLISSIONS PER PARTICLE
        WITH RELATIVE DEVIATION > .01000 ...............   .16432D-01
        WITH RELATIVE DEVIATION > .05000 ...............   .46948D-02
        WITH RELATIVE DEVIATION > .15000 ...............   .23474D-02
        WITH RELATIVE DEVIATION > .50000 ...............   .00000D+00
      AVERAGE VALUE OF ECCENTRICITY PARAMETER B/B(90) ... 8.76213D+04
      MINIMUM VALUE OF ECCENTRICITY PARAMETER B/B(90) ... 1.66466D-01
      MAXIMUM VALUE OF ECCENTRICITY PARAMETER B/B(90) ... 1.79038D+06
THIN LENS(2) AT Z (IN M) ............................. 4.80000D-01
      FOCAL LENGTH (IN M) .............................. 1.60000D-01
      SPHERICAL ABERRATION COEFFICIENT (IN M) .......... 1.60000D-01
      CHROMATIC ABERRATION COEFFICIENT (IN M) .......... 8.00000D-02
      ROTATIONAL DISTORSION COEFFICIENT (IN RAD) ....... 0.00000D+00
      ROTATIONAL CHROMATIC ABERRATION COEFF. (IN RAD) ... 0.00000D+00
DRIFT2: ANALYTICAL CALCULATION OF TRAJECTORIES
      DRIFT SECTION NUMBER .............................       4
      START DRIFT LENGTH AT Z0 (IN M) .................. 4.80000D-01
      END DRIFT LENGTH AT Z1 (IN M) .................... 6.80000D-01
      BEAM POTENTIAL (IN V) ............................ 1.00000D+05
      TIME OF FLIGHT FROM Z0 TO Z1 (IN S) .............. 1.06637D-09
      MUTUAL INTERACTION (1,2=ON, 0=OFF) ...............       1
      PROCESSING OF END-EFFECTS OF SAMPLE (1=YES,0=NO) ..      0
      INTERACTION RANGE LIMITATION (1=YES,0=NO) ........       0
      AVERAGE NUMBER OF CALCULATIONS USING FIRST ORDER
        PERTURBATION THEORY PER PARTICLE ............... 8.49441D+02
      AVERAGE NUMBER OF CALCULATIONS USING COMPLETE
        COLLISION DYNAMICS  PER PARTICLE ............... 2.34742D-03
      AVERAGE NUMBER OF CALCULATIONS USING FULL
        COLLISION DYNAMICS  PER PARTICLE ............... 1.55634D+00
```

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        AVERAGE NUMBER OF STRONG COLISSIONS PER PARTICLE
          WITH RELATIVE DEVIATION > .01000 ................  .30516D-01
          WITH RELATIVE DEVIATION > .05000 ................  .11737D-01
          WITH RELATIVE DEVIATION > .15000 ................  .46948D-02
          WITH RELATIVE DEVIATION > .50000 ................  .00000D+00
        AVERAGE VALUE OF ECCENTRICITY PARAMETER B/B(90) ... 1.46532D+06
        MINIMUM VALUE OF ECCENTRICITY PARAMETER B/B(90) ... 8.73906D-02
        MAXIMUM VALUE OF ECCENTRICITY PARAMETER B/B(90) ... 2.25909D+07
THIN LENS(2) AT Z (IN M) ............................ 6.80000D-01
        FOCAL LENGTH (IN M) ............................. 4.00000D-02
        SPHERICAL ABERRATION COEFFICIENT (IN M) .......... 4.00000D-02
        CHROMATIC ABERRATION COEFFICIENT (IN M) .......... 2.00000D-02
        ROTATIONAL DISTORSION COEFFICIENT (IN RAD) ....... 0.00000D+00
        ROTATIONAL CHROMATIC ABERRATION COEFF. (IN RAD) ... 0.00000D+00
DRIFT2: ANALYTICAL CALCULATION OF TRAJECTORIES
        DRIFT SECTION NUMBER .............................          5
        START DRIFT LENGTH AT Z0 (IN M) .................. 6.80000D-01
        END DRIFT LENGTH AT Z1 (IN M) .................... 7.20000D-01
        BEAM POTENTIAL (IN V) ............................ 1.00000D+05
        TIME OF FLIGHT FROM Z0 TO Z1 (IN S) .............. 2.13273D-10
        MUTUAL INTERACTION (1,2=ON, 0=OFF) ...............          1
        PROCESSING OF END-EFFECTS OF SAMPLE (1=YES,0=NO) ..        0
        INTERACTION RANGE LIMITATION (1=YES,0=NO) ........        0
        AVERAGE NUMBER OF CALCULATIONS USING FIRST ORDER
          PERTURBATION THEORY PER PARTICLE ............... 8.49279D+02
        AVERAGE NUMBER OF CALCULATIONS USING COMPLETE
          COLLISION DYNAMICS  PER PARTICLE ............... 0.00000D+00
        AVERAGE NUMBER OF CALCULATIONS USING FULL
          COLLISION DYNAMICS  PER PARTICLE ............... 1.72066D+00
        AVERAGE NUMBER OF STRONG COLISSIONS PER PARTICLE
          WITH RELATIVE DEVIATION > .01000 ................  .46948D-02
          WITH RELATIVE DEVIATION > .05000 ................  .00000D+00
          WITH RELATIVE DEVIATION > .15000 ................  .00000D+00
          WITH RELATIVE DEVIATION > .50000 ................  .00000D+00
        AVERAGE VALUE OF ECCENTRICITY PARAMETER B/B(90) ... 1.34752D+06
        MINIMUM VALUE OF ECCENTRICITY PARAMETER B/B(90) ... 1.22163D+00
        MAXIMUM VALUE OF ECCENTRICITY PARAMETER B/B(90) ... 2.86320D+07


STOREC: STORES THE COORDINATES OF PARTICLES TO FILE (FORMAT=1)



        ****      RESULTS OF MONTE CARLO CALCULATION      ****


            ****       FROM SUBROUTINE TBR (T1)     ****


RADIAL INTERACTION-DISPLACEMENT DISTRIBUTION :
        TOTAL NUMBER OF PARTICLES .........................      5101
        NUMBER OF DIVISIONS IN HISTOGRAM ..................        50
        DIVISION-WIDTH (IN M) ............................ 1.77732D-09
EFFECTIVE SPATIAL BROADENING IN PLANE OF BEST FOCUS :
        Z-COORDINATE OF REFERENCE PLANE (IN M) ........... 7.20000D-01
        AXIAL DEFOCUS RELATIVE TO REFERENCE PLANE (IN M) .. 0.00000D+00
        SUB-ENSEMBLE SIZE FOR ESTIMATE OF STATISTICAL ERROR       71
        NUMBER OF SUB-ENSEMBLES ..........................        71
        RELATIVE STATISTICAL ERROR IN RMS R (3*RMS-VALUE) . 6.99750D-02
        RELATIVE STATISTICAL ERROR IN 50%-FWR (3*RMS-VALUE) 3.87982D-02
        AVERAGE X (IN M) ................................. 3.28662D-08
        AVERAGE Y (IN M) ................................. 3.31473D-08
        RMS X (IN M) ..................................... 2.50085D-08
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        RMS Y (IN M) ...................................... 2.41748D-08
        RMS R (IN M) ...................................... 3.47829D-08
        10%-FW R (IN M) ................................... 4.25998D-08
        30%-FW R (IN M) ................................... 7.67243D-08
        50%-FW R (IN M) ................................... 1.02039D-07
        70%-FW R (IN M) ................................... 1.25662D-07
        90%-FW R (IN M) ................................... 1.58259D-07
        FWHM X (IN M) ..................................... 1.11912D-07
        FWHM Y (IN M) ..................................... 1.13402D-07
        (FWHMX + FWHMY)/2 (IN M) .......................... 1.12657D-07
        FWHM R (IN M) ..................................... 1.45348D-07
LEAST SQUARE FIT OF SPATIAL DISTRIBUTION IN PLANE OF FOCUS
WITH A POLYNOMIAL FUNCTION OF   6 TERMS :
        DIST(DR)  =  5.17444D+08 * ( 1.00000D+00 +
                               2.86979D+00 * (2*DR/FWHMR)** 2 +
                              -1.43804D+01 * (2*DR/FWHMR)** 4 +
                               2.38176D+01 * (2*DR/FWHMR)** 6 +
                              -1.74368D+01 * (2*DR/FWHMR)** 8 +
                               4.63002D+00 * (2*DR/FWHMR)**10 +


            ****     FROM SUBROUTINE RECTBR (T2)    ****


RECTANGULAR SPATIAL DISTRIBUTION :
        TOTAL NUMBER OF PARTICLES ........................      5101
        NUMBER OF DIVISIONS IN TOTAL HISTOGRAM ...........       100
        NUMBER OF DIVISIONS IN HISTOGRAM OF THE EDGE.......         2
        DIVISION-WIDTH (IN M) ............................ 1.28173D-06
AVERAGE AMPLITUDES, SHIFTS AND INTERVALS USED FOR L-S FITS:
        A0X   = 5.22784D+01   XW0   = 1.24327D-04   XW1  = 1.26880D-04
        DSHIFTX= 2.61392D+01   SHIFTX = 1.27624D-06
        A0Y   = 5.20510D+01   YW0   = 1.25609D-04   YW1  = 1.25775D-04
        DSHIFTY= 2.60255D+01   SHIFTY = 8.31188D-08
EFFECTIVE SPATIAL BROADENING IN PLANE OF BEST FOCUS :
        Z-COORDINATE OF REFERENCE PLANE (IN M) ........... 7.20000D-01
        AXIAL DEFOCUS RELATIVE TO REFERENCE PLANE (IN M) . 0.00000D+00
        AVERAGE X (IN M) .................................-1.41653D-06
        AVERAGE Y (IN M) ................................. 2.58354D-07
        HWHM X (IN M) .................................... 1.24847D-04
        HWHM Y (IN M) .................................... 1.26054D-04
        D2575 X (IN M) ................................... 3.57938D-07
        D2575 Y (IN M) ................................... 2.38421D-07
        D2575 AVERAGE (IN M) ............................. 2.98180D-07
        D1288 X (IN M) ................................... 5.70057D-07
        D1288 Y (IN M) ................................... 3.83964D-07
        D1288 AVERAGE (IN M).............................. 4.77011D-07
        WARNING: ACCURACY OF EDGE-WIDTH IS LIMITED BY
                 THE DIVISION WIDTH OF THE HISTOGRAM
LEAST SQUARE FIT OF SPATIAL DISTRIBUTION IN PLANE OF FOCUS
WITH A POLYNOMIAL FUNCTION OF   6 TERMS :
        DIST(X)=-1.5309D+01*( 1.0000D+00 +
                        1.7469D-01*(2*(X-1.2560D-04)/D2575X)**( 1/ 1) +
                       -1.5236D-01*(2*(X-1.2560D-04)/D2575X)**( 2/ 1) +
                       -8.8871D-03*(2*(X-1.2560D-04)/D2575X)**( 3/ 1) +
                       -1.1343D-04*(2*(X-1.2560D-04)/D2575X)**( 4/ 1) +
                       -8.9437D-05*(2*(X-1.2560D-04)/D2575X)**( 5/ 1) +
        DIST(Y)= 5.1102D+01*( 1.0000D+00 +
                       -5.3050D-02*(2*(Y-1.2569D-04)/D2575Y)**( 1/ 1) +
                       -3.7516D-02*(2*(Y-1.2569D-04)/D2575Y)**( 2/ 1) +
                        4.9905D-04*(2*(Y-1.2569D-04)/D2575Y)**( 3/ 1) +
```

```
                      1.7295D-06*(2*(Y-1.2569D-04)/D2575Y)**( 4/ 1) +
                      7.7959D-06*(2*(Y-1.2569D-04)/D2575Y)**( 5/ 1) +


         ****      FROM SUBROUTINE TBR (T1)    ****


RADIAL INTERACTION-DISPLACEMENT DISTRIBUTION :
     TOTAL NUMBER OF PARTICLES ........................    5101
     NUMBER OF DIVISIONS IN HISTOGRAM ..................     50
     DIVISION-WIDTH (IN M) ........................... 7.90454D-10
EFFECTIVE SPATIAL BROADENING IN PLANE OF BEST FOCUS :
     Z-COORDINATE OF REFERENCE PLANE (IN M) ........... 7.20000D-01
     AXIAL DEFOCUS RELATIVE TO REFERENCE PLANE (IN M) .. 1.83343D-05
     FOCUS CRITERION USED (1=FW50, 2=FW90, 3=FWHM)......       1
     SUB-ENSEMBLE SIZE FOR ESTIMATE OF STATISTICAL ERROR     71
     NUMBER OF SUB-ENSEMBLES ..........................      71
     RELATIVE STATISTICAL ERROR IN RMS R (3*RMS-VALUE) . 1.09853D-01
     RELATIVE STATISTICAL ERROR IN 50%-FWR (3*RMS-VALUE) 9.15788D-02
     AVERAGE X (IN M) .................................. 2.03280D-08
     AVERAGE Y (IN M) .................................. 2.00341D-08
     RMS X (IN M) ..................................... 1.94634D-08
     RMS Y (IN M) ..................................... 1.83507D-08
     RMS R (IN M) ..................................... 2.67502D-08
     10%-FW R (IN M) .................................. 1.43658D-08
     30%-FW R (IN M) .................................. 2.66082D-08
     50%-FW R (IN M) .................................. 3.86798D-08
     70%-FW R (IN M) .................................. 5.41832D-08
     90%-FW R (IN M) .................................. 8.86886D-08
     FWHM X (IN M) .................................... 3.63388D-08
     FWHM Y (IN M) .................................... 3.48843D-08
     (FWHMX + FWHMY)/2 (IN M) ......................... 3.56116D-08
     FWHM R (IN M) .................................... 3.01493D-08
LEAST SQUARE FIT OF SPATIAL DISTRIBUTION IN PLANE OF FOCUS
WITH A POLYNOMIAL FUNCTION OF   6 TERMS :
     DIST(DR)  =  2.86021D+09 * ( 1.00000D+00 +
                               -7.71045D-01 * (2*DR/FWHMR)** 2 +
                                3.51078D-01 * (2*DR/FWHMR)** 4 +
                               -9.15120D-02 * (2*DR/FWHMR)** 6 +
                                1.19775D-02 * (2*DR/FWHMR)** 8 +
                               -6.05248D-04 * (2*DR/FWHMR)**10 +


         ****     FROM SUBROUTINE RECTBR (T2)    ****


RECTANGULAR SPATIAL DISTRIBUTION :
     TOTAL NUMBER OF PARTICLES ........................    5101
     NUMBER OF DIVISIONS IN TOTAL HISTOGRAM ...........     100
     NUMBER OF DIVISIONS IN HISTOGRAM OF THE EDGE.......      5
     DIVISION-WIDTH (IN M) ........................... 1.27758D-06
AVERAGE AMPLITUDES, SHIFTS AND INTERVALS USED FOR L-S FITS:
     A0X   = 5.22979D+01   XW0   = 1.20093D-04   XW1   = 1.25940D-04
     DSHIFTX= 2.61489D+01   SHIFTX = 2.92362D-06
     A0Y   = 5.20510D+01   YW0   = 1.25203D-04   YW1   = 1.25475D-04
     DSHIFTY= 2.60255D+01   SHIFTY = 1.36095D-07
EFFECTIVE SPATIAL BROADENING IN PLANE OF BEST FOCUS :
     Z-COORDINATE OF REFERENCE PLANE (IN M) .......... 7.20000D-01
     AXIAL DEFOCUS RELATIVE TO REFERENCE PLANE (IN M) . 1.83343D-05
     AVERAGE X (IN M) ................................-1.41688D-06
     AVERAGE Y (IN M) ................................. 2.57812D-07
     HWHM X (IN M) .................................... 1.23833D-04
     HWHM Y (IN M) .................................... 1.25916D-04
```

```
    D2575 X (IN M) .................................. 3.25870D-06
    D2575 Y (IN M) .................................. 5.03651D-07
    D2575 AVERAGE (IN M) ............................ 1.88118D-06
    WARNING: ACCURACY OF EDGE-WIDTH IS LIMITED BY
             THE DIVISION WIDTH OF THE HISTOGRAM
 LEAST SQUARE FIT OF SPATIAL DISTRIBUTION IN PLANE OF FOCUS
 WITH A POLYNOMIAL FUNCTION OF   6 TERMS :
    DIST(X)= 3.9179D+01*( 1.0000D+00 +
                         -7.1622D-01*(2*(X-1.2302D-04)/D2575X)**( 1/ 1) +
                         -2.7501D-02*(2*(X-1.2302D-04)/D2575X)**( 2/ 1) +
                          2.7505D-01*(2*(X-1.2302D-04)/D2575X)**( 3/ 1) +
                         -2.1912D-03*(2*(X-1.2302D-04)/D2575X)**( 4/ 1) +
                         -4.0319D-02*(2*(X-1.2302D-04)/D2575X)**( 5/ 1) +
    DIST(Y)= 5.0621D+01*( 1.0000D+00 +
                         -9.9775D-02*(2*(Y-1.2534D-04)/D2575Y)**( 1/ 1) +
                         -7.9398D-02*(2*(Y-1.2534D-04)/D2575Y)**( 2/ 1) +
                          1.5257D-02*(2*(Y-1.2534D-04)/D2575Y)**( 3/ 1) +
                         -9.1954D-04*(2*(Y-1.2534D-04)/D2575Y)**( 4/ 1) +
                          1.7939D-05*(2*(Y-1.2534D-04)/D2575Y)**( 5/ 1) +


          ****        FROM SUBROUTINE SYMEBR       ****


 ENERGY DISTRIBUTION :
    TOTAL NUMBER OF PARTICLES ......................      5101
    NUMBER OF DIVISIONS IN HISTOGRAM ...............        50
    DIVISION-WIDTH (IN EV) .......................... 2.82370D-02
 ENERGY MEASURES (IN EV) REFER TO LAST Z-COORDINATE :
    SUB-ENSEMBLE SIZE FOR ESTIMATE OF STATISTICAL ERROR       71
    NUMBER OF SUB-ENSEMBLES .........................        71
    RELATIVE STATISTICAL ERROR IN RMS (3*RMS-VALUE) ... 3.07128D-02
    RELATIVE STATISTICAL ERROR IN 50%-FW (3*RMS-VALUE) 5.84101D-02
    AVERAGE ENERGY /TOTAL VELOCITY/ ................... 1.00001D+05
    AVERAGE ENERGY /Z-COMPONENT OF VELOCITY/ ......... 1.00000D+05
    RMS OF ENERGY DISTRIBUTION ....................... 7.56611D-01
    RMS OF ENERGY DISTRIBUTION /Z-COMP. OF VELOCITY/ .. 4.87537D-01
    10% FW ENERGY DISTRIBUTION /Z-COMP. OF VELOCITY/... 1.18055D-01
    30% FW ENERGY DISTRIBUTION /Z-COMP. OF VELOCITY/... 3.67281D-01
    50% FW ENERGY DISTRIBUTION /Z-COMP. OF VELOCITY/... 6.33889D-01
    70% FW ENERGY DISTRIBUTION /Z-COMP. OF VELOCITY/... 9.82394D-01
    90% FW ENERGY DISTRIBUTION /Z-COMP. OF VELOCITY/... 1.58634D+00
    FWHM  ENERGY DISTRIBUTION  /Z-COMP. OF VELOCITY/... 1.09978D+00
 LEAST SQUARE FIT OF FOLDED ENERGY DISTRIBUTION
 WITH A POLYNOMIAL FUNCTION OF   6 TERMS:
    DIST(DE)  =  2.43090D+02 * ( 1.00000D+00 +
                              -6.81526D-01 * (2*DE/FWHM)** 2 +
                               2.14593D-01 * (2*DE/FWHM)** 4 +
                              -3.60232D-02 * (2*DE/FWHM)** 6 +
                               3.00989D-03 * (2*DE/FWHM)** 8 +
                              -9.52536D-05 * (2*DE/FWHM)**10 +


          ****      PROCESSING OF COORDINATES      ****


 PROCCO1: COMPENSATION OF Z-DEPENDENCY IN Z-COMPONENT OF VELOCITY
    NOMINAL FRACTION OF PARTICLES TO BE USED IN FIT ... 8.00000D-01
    NUMBER OF PARTICLES USED IN FIT PERTURBED COORD. ..      4081
    AVERAGE Z-POSITION <Z> (IN M) .................... 7.20003D-01
    AVERAGE Z-VELOCITY <Vz> (IN M/S) ................. 1.87553D+08
    Z-POSITION RANGE PERTURBED COORDINATES Rz (IN M) .. 4.10103D-03
    Z-VELOCITY RANGE PERTURBED COORDINATES RVz (IN M/S) 5.15479D+03
```

```
NUMBER OF DIVISIONS IN HISTOGRAM ..................        10
NUMBER OF TERMS IN FIT FUNCTION PERTURBED COORD. ..         1
NUMBER OF PARTICLES USED IN FIT UNPERTURBED COORD.      4081
Z-POSITION RANGE UNPERTURBED COORDINATES Rzu (IN M) 4.10088D-03
Z-VELOCITY RANGE UNPERTURBED COORDINATES (IN M/S) . 3.23511D+03
NUMBER OF TERMS IN FIT FUNCTION UNPERTURBED COORD.         1
LEAST SQUARE FIT OF Z-VELOCITY AS FUNCTION OF Z-POSITION :
- FOR PERTURBED COORDINATES :
  (Vz(Z)-<Vz>)/RVz =  2.87981D-02 * [ (Z-<Z>)/Rz ]** 1 +
- FOR UNPERTURBED COORDINATES :
  (Vz(Z)-<Vz>)/RVz = -3.61985D-03 * [ (Z-<Z>)/Rzu ]** 1 +


     ****          FROM SUBROUTINE SYMEBR       ****


ENERGY DISTRIBUTION :
    TOTAL NUMBER OF PARTICLES .........................      5101
    NUMBER OF DIVISIONS IN HISTOGRAM ..................        50
    DIVISION-WIDTH (IN EV) ............................ 2.76034D-02
ENERGY MEASURES (IN EV) REFER TO LAST Z-COORDINATE :
    SUB-ENSEMBLE SIZE FOR ESTIMATE OF STATISTICAL ERROR       71
    NUMBER OF SUB-ENSEMBLES ...........................        71
    RELATIVE STATISTICAL ERROR IN RMS (3*RMS-VALUE) ... 3.13253D-02
    RELATIVE STATISTICAL ERROR IN 50%-FW (3*RMS-VALUE) 6.63267D-02
    AVERAGE ENERGY /TOTAL VELOCITY/ ................... 1.00001D+05
    AVERAGE ENERGY /Z-COMPONENT OF VELOCITY/ .......... 1.00000D+05
    RMS OF ENERGY DISTRIBUTION ........................ 7.49078D-01
    RMS OF ENERGY DISTRIBUTION /Z-COMP. OF VELOCITY/ .. 4.76108D-01
    10% FW ENERGY DISTRIBUTION /Z-COMP. OF VELOCITY/... 1.19110D-01
    30% FW ENERGY DISTRIBUTION /Z-COMP. OF VELOCITY/... 3.59825D-01
    50% FW ENERGY DISTRIBUTION /Z-COMP. OF VELOCITY/... 6.28550D-01
    70% FW ENERGY DISTRIBUTION /Z-COMP. OF VELOCITY/... 9.55498D-01
    90% FW ENERGY DISTRIBUTION /Z-COMP. OF VELOCITY/... 1.54468D+00
    FWHM  ENERGY DISTRIBUTION  /Z-COMP. OF VELOCITY/... 1.08720D+00
LEAST SQUARE FIT OF FOLDED ENERGY DISTRIBUTION
WITH A POLYNOMIAL FUNCTION OF   6 TERMS:
    DIST(DE)  =  2.41870D+02 * ( 1.00000D+00 +
                               -6.76620D-01 * (2*DE/FWHM)** 2 +
                                2.08490D-01 * (2*DE/FWHM)** 4 +
                               -3.48172D-02 * (2*DE/FWHM)** 6 +
                                3.04344D-03 * (2*DE/FWHM)** 8 +
                               -1.09875D-04 * (2*DE/FWHM)**10 +


STOREP: STORES THE PROJECTED POSITIONS OF PARTICLES TO FILE (FORMAT=1)
    Z-COORDINATE OF REFERENCE PLANE (IN M) ........... 7.20000D-01


STOREP: STORES THE PROJECTED POSITIONS OF PARTICLES TO FILE (FORMAT=1)
    Z-COORDINATE OF REFERENCE PLANE (IN M) ........... 7.20018D-01


START PROGRAM:  0:30:52 ON  7/10/2003
END PROGRAM :  0:31:32 ON  7/10/2003
RUN TIME    :     0 HOUR,  0 MIN AND 40 S
```

Appendix B.   INTERAC screen shots

Worksheet Dashboard

Dashboard | System | Section | MC_in | MC_out | MC_edi | MC_sdi | MC_pos | MC_cor | PlotDis | PlotPos | PlotCor | Runs | Results | PlotRuns1 | PlotRuns2 | About | Settings

Full Screen On/Off | Expand | Collapse | Zoom

Interac Dashboard   **MonTec**
Version 1.7, Licensed to Caneval BV, 19/1/2004   Particle Optics Simulation Tools

MC files for data analysis	MC input files drive & directory	C:	\MonTec\Demo\In	Same as	Browse
	MC output files drive & directory	C:	\MonTec\Demo\Out	run files	Browse
Selected series	Series ID (or "All" for all runs in all series)	Systems	Previous series	Next series	Go to 'Runs' specification area
	Number of runs in series	6			
Selected run	Selected run no.	1	Previous run	Next run	
	Data file identifyer	DEMO1	Run 1 - Series Systems :		
	System file identifyer	DEMO1	DEMO1.DAT & DEMO1.SYS		

Input and Output File Names for Selected Run: 1

File type		Extension	Filename	Exist ?
Input files	MC-data input file	DAT	DEMO1.DAT	TRUE
	MC-system input file	SYS	DEMO1.SYS	TRUE
Output files	MC- coordinates input/output file	COR	DEMO1.COR	TRUE
	MC- general output file	OUT	DEMO1.OUT	TRUE
	MC-energy distribution output file	EDI	DEMO1.EDI	TRUE
	MC-spatial distribution output file	SDI	DEMO1.SDI	TRUE
	MC- radial positions output file	POS	DEMO1.POS	TRUE
Workload execution command line	RUN MC C:\MonTec\Demo\In\DEMO1 * WorkId C:\MonTec\Demo\Out\DEMO1			

Monte Carlo Simulation (Automatic MC Parameters: Off)

Export input file MC DAT	☑	Export files	Add selected run to workload	Run job	Workload started: C:\MonTec\MC\WorkId.BAT
Export input file MC SYS	☑		Add selected series to workload	Run workload	
Copy system data first ?	☑	Edit files	Edit workload	Clear workload	C:\...	

Data Analysis for Selected Run: 1

Input files	☑	Import "checked" files	Import MC DAT & MC SYS files	Show system	Clear imported data	Completed - Run 1
Copy input data to system ?	☑					
General output file	☑		Import MC OUT file			Completed - Run 1
Energy distribution file	☑		Import MC EDI file			Completed - Run 1
Maintain current scale ?	☐					
Spatial distribution file	☑		Import MC SDI file			Completed - Run 1
Maintain current scale ?	☐					
Positions file	☑		Import MC POS file			Completed - Run 1
Maintain current scale ?	☐					
Max no particles (<60000)	5,000					
Co-ordinates file	☑		Import MC COR file			Completed - Run 1
Maintain current scale ?	☐					
Max no particles (<60000)	5,000					

Data Storage to Worksheet 'Results'

| Extrac key results from OUT files ? | ☑ | Store data for selected run | Store data for selected series | Clear all data from memory | MC input & output data and analytical calculation stored - Run 1 |
| Execute analytical calculation ? | ☑ | | | | |

Spreadsheet Management

| User data and settings: | | Reset all screens | Clear all user data | Reset all model parameters | Reset entire spreadsheet | Task abandoned |
| Clear worksheet 'Runs' data? | ☑ | | | | | |

Worksheet Dashboard with MC command window and system plot window

MonTec
Particle Optics Simulation Tools

C:\WINDOWS\System32\cmd.exe

```
┌─────────────────── PROGRAM ───────────────────┐
│   Monte Carlo Simulation of Particle Beam Systems │
│        (C) Caneval B.V., 1989-2004               │
│                            Version 3.3           │
└──────────────────────────────────────────────────┘

┌────────────────────── JOB ────────────────────┐
│ System Input File: C:\MONTEC\DEMO\IN\JEOL.SYS   │
│ Data Input File:   C:\MONTEC\DEMO\IN\JEOL.DAT   │
│ Job Started at:    11:52 on 27/ 1/2004          │
└──────────────────────────────────────────────────┘

┌─────────────────── PROCESS ───────────────────┐
│ Seeds to Go:  │ Activity: Started at: │ Beam Section: │
│    12         │ DRIFT2        11:52   │     3         │
```

Runs'
nTec\MC | Browse

nTec\Demo\In | Same as | Browse
nTec\Demo\Out | run files | Browse

evious series | Next series | Go to 'Runs' specification area
Previous run | Next run

Run 30 - Series Systems : JEOL.DAT & JEOL.SYS

0
name | Exist ?

Close | System file: JEOL.SYS | Normal Size

Key figures from MC data file JEOL.DAT and MC system file JEOL.SYS and derived data from analytical model:

Source / Target:	Particles mass and charge of electron	**Optical components:**	Number of beam sections = 6
	Axial location source = 0.0000E+00 (m) / target = 3.8100E-01 (m)		Number of lenses / quadrupoles = 3 / 0
	Beam current at source = 1.0000E-05 (A) / at target 1.6035E-09 (A)		Number of deflectors = 0
	Beam voltage at source = 5.0000E+03 (V) / at target 5.0000E+04 (V)		Number of apertures = 2
	FWHM energy spread at source 3.7223E-01 eV (Lorentizian distribution)	**MC parameters:**	NSAM at source = 500000 / at target = 80
	Circular Gaussian source surface with XHW=YHW=1.5000E-08 m		NSEED = 13, NTOT at target = 1042
	Circular uniform angular distribution with AHW = 1.2620E-01 (Rad)	**Ray-tracing algorithm:**	6 x DRIFT2;
Interaction per section:	1:Off2:Off3:On, 4:On, 5:On, 6:On,	**Estimated MC run-time:**	1 hour,4 min and 54 s (Order of magnitude)
Crossovers at:	-2.65E-04, 4.95E-02, 2.05E-01, 3.81E-01 (m)	**Transverses magnifications in conjugated planes:**	
Source conjug. planes at:	0.00E+00, 4.95E-02, 2.05E-01, 3.81E-01 (m)	1.00E+00, 4.27E-01, 8.11E-02, 8.10E-03 (source to conjugated plane)	
Target conjug. planes at:	3.81E-01, 2.05E-01, 4.96E-02, 1.92E-04 (m)	1.00E+00, 9.99E-02, 1.90E-02, 8.43E-03 (conjugated plane to target)	

Worksheet Runs (top-section)

Full Screen On/Off | Zoom — **MC Run Jobs Specification** — Go to 'Dashboard' | Restore Defaults

Run no.	Series ID	DAT file minus ext. (max 10 char.)	SYS file minus ext. (max 10 char.)	I (uA)	V (10 kV)				NSAM	NSEED	DRIFTX			Remarks
		MC run & series specification		**System Input**					**MC program parameter setting**					
1	Default	DEMO1	DEMO1	10	100				Automatic		DRIFT2			
2	D1-test	DEMO1T1	DEMO1	100	100				200	100	DRIFT2			
3	D1-test	DEMO1T2	DEMO1	100	100				500	40	DRIFT2			
4	D1-test	DEMO1T3	DEMO1	100	100				1000	20	DRIFT2			
5	D1-test	DEMO1T4	DEMO1	100	100				2000	10	DRIFT2			
6	D1-test	DEMO1T5	DEMO1	100	100				5000	4	DRIFT2			
7	D1-test	DEMO1T6	DEMO1	100	100				10000	2	DRIFT2			
8	D1-test	DEMO1T7	DEMO1	100	100				20000	1	DRIFT2			
9	D1-IS	DEMO1I1	DEMO1	1	100				Automatic		DRIFT2			
10	D1-IS	DEMO1I2	DEMO1	2	100				Automatic		DRIFT2			
11	D1-IS	DEMO1I5	DEMO1	5	100				Automatic		DRIFT2			
12	D1-IS	DEMO1I10	DEMO1	10	100				Automatic		DRIFT2			
13	D1-IS	DEMO1I20	DEMO1	20	100				Automatic		DRIFT2			
14	D1-IS	DEMO1I50	DEMO1	50	100				Automatic		DRIFT2			
15	D1-IS	DEMO1I100	DEMO1	100	100				Automatic		DRIFT2			
16	D1-VS	DEMO1V5	DEMO1	10	5				Automatic		DRIFT2			
17	D1-VS	DEMO1V10	DEMO1	10	10				Automatic		DRIFT2			
18	D1-VS	DEMO1V20	DEMO1	10	20				Automatic		DRIFT2			
19	D1-VS	DEMO1V50	DEMO1	10	50				Automatic		DRIFT2			
20	D1-VS	DEMO1V100	DEMO1	10	100				Automatic		DRIFT2			
21	D1-VS	DEMO1V200	DEMO1	10	200				Automatic		DRIFT2			
22	D1-IS-D1	DEMO1I1D	DEMO1D1	1	100				Automatic		DRIFT1			
23	D1-IS-D1	DEMO1I10D	DEMO1D1	10	100				Automatic		DRIFT1			
24	D1-IS-D1	DEMO1I100D	DEMO1D1	100	100				Automatic		DRIFT1			
25	Systems	SCALPEL	SCALPEL						Automatic		DRIFT2			Identical to default series
26	Systems	IMS	IMS						Automatic		DRIFT2			
27	Systems	IBMEL3	IBMEL3						Automatic		DRIFT2			
28	Systems	AEBLE150	AEBLE150						Automatic		DRIFT2			
29	Systems	DualGA	DualGA						Automatic		DRIFT2			
30	Systems	JEOL	JEOL						Automatic		DRIFT2			
31														
32														

Worksheet System ('Set-up for system input' view, top-section)

Expand all areas	Collapse all areas	Full Screen On/Off	Unlockcharts	Zoom	**System Definition & Calculations**	Increase abs	Decrease abs	1.0000E-02	Increase %	Decrease %	0.0001%
Expand	Collapse	Copy data from MC_in	Copy system data to MC_in	**System plot: Principal Rays in Total System - X direction**	Set-up screen for system input	Reset for new system	Load demo system
Scale plot	Show system plot in separate window

System file: DEMO1.SYS

Legend: Straightline / Dashed axis: Interaction on / off

| Expand | Collapse | **Source Properties** |

Category	Geometric properties	Identifier	Unit	Value	Beam properties	Identifier	Unit	Value
	X-coordinate of source centre	XCTR	m	0.0000E+00	Particle mass	PMASS / PM	kg	9.1096E-31
	Y-coordinate of source centre	YCTR	m	0.0000E+00	Absolute value of particle charge in elementary charge units	NCHRG / PQ	-	1.0000E+00
Source Properties	Spatial distribution type (1=Circular uniform, 2= Circular Gaussian, 3= Rectangular)	IDS	-	2	Beam current at emission	BI	A	1.0000E-05
	Source half width in X-direction (HWHM)	XHW	m	8.0000E-05	FWHM energy spread at emission	FWE	eV	1.0000E+00
	Source half width in Y-direction (HWHM)	YHW	m	8.0000E-05	Type of energy distribution (1=Uniform, 2=Gaussian, 3=Lorentzian)	IDE	-	2
	Angular distribution type (1=Circular uniform, 2= Circular Gaussian, 3= MB thermal distribution)	IDA	-	1	Cathode temperature	TCA	K	2.5000E+03
	Beam semi angle HWHM	AHW	Rad	5.0000E-03	Beam semi angle HWHM corresponding to Cathod temperature	AHW	Rad	1.728E-03

| Expand | Collapse | **Optical Components and Drift Sections** |

Specification / value by beam section

Category	Variable description	Identifier	Unit	1	2	3	4	5	6	7	8	9	10	Target
Beam sections	Particle interaction switch (0=Off, 1=On)	INTER	-	0	0	1	1	1						
	Axial coordinate at start of section (first = source, last = target)	Z0	m	0.0000E+00	1.6000E-01	3.2000E-01	4.8000E-01	6.8000E-01						7.2000E-01
	Beam potential at start of section (= value at end previous section)	BV0	V	1.0000E+05										
Collapse	Active (1=Yes, 0= No)	lens-switch	-		1		1	1						
	X-coordinate of lens centre	XCTR	m											
	Y-coordinate of lens centre	YCTR	m											
Lenses (at start of beam section)	Focal distance F	F	m		1.6000E-01		1.6000E-01	4.0000E-02						
	Spherical aberration coefficient (object side, infinit magnification)	CS(Obj,inf)	m		1.6000E-01		1.6000E-01	4.0000E-02						
	Chromatic aberration coefficient (object side, infinit magnification)	CC(Obj,inf)	m		8.0000E-02		8.0000E-02	2.0000E-02						
	Coefficient of rotational distorsion (magnetic lens)	RD	Rad											
	Coefficient of chromatic error in rotational distorsion (magnetic lens)	RC	Rad											
Collapse	Active (1=Yes, 0= No)	Defl.-switch	-											
Deflectors (at start of beam section)	Angular deflection in X-direction	AX	m											
	Angular deflection in Y-direction	AY	m											
	Dispersion (chromatic aberration) coefficient	DC	Rad											
Collapse	Active (1=Yes, 0= No)	Apert.-switch	-		1	1								
Apertures (at start of beam section)	X-coordinate of lens centre	XCTR	m											
	Y-coordinate of lens centre	YCTR	m											
	Half width in X-direction	XHM	m		6.6000E-04	5.0000E-04								
	Half width in Y-direction	YHM	m		6.6000E-04	5.0000E-04								
	Shape index (1=Circular aperture, 2= Square aperture)	ISHP	-		2	2								

Worksheet System ('Monte Carlo Simulation Parameters' section)

| Expand | Collapse | | Monte Carlo Simulation Parameters | | | | | | | | Automatic: | Off | On | Off |

Key MC data input file parameters (See worksheet MC_in for full details) — **MC system input file commands for data analysis and storage** (See worksheet MC_in for full details)

MC input files settings	ICONS	NDE	NDT1	NDT2	ISTOREE	ISTORET1	ISTORET2	IMT1	IMT2	Coordinates storage/retrieval (1=Yes, 0=No)		Radial positions analysis and storage (0=No, 1= in target plane, 2= in plane of best focus, 3=in target and plane of best focus)				Energy distribution analysis (0=No, 1=without PROCCO, 2=without and with PROCCO)	
	2	50	50	100	1	1	1	-1	1								
	INTER	NSAM	NSEED	NFIELD	NSTEP	ISTEPA	IRLIM	NINT	IPROC	STOREC	READC	TBR	RNDTBR	RECTBR	STOREP	SYMEBR	ASYEBR
	1	1,700	6	10,000	2,000	1	0	1,000	0	1	0	3	0	3	3	2	0

Ray tracing algorithm and run-time estimate	Beam section	1	2	3	4	5	6	7	8	9	10	Target
	Ray tracing algorithm by beam section (1=DRIFT1,2=DRIFT2,3=DRIFT3; 2=Default)	2	2	2	2	2						
	Number of particles in the sample by beam section (NSAM)	1,700	1,473	846	846	846						846
	Total number of particles by beam section in all seeds (NTOT = NSAM X NSEED)	10,200	8,839	5,073	5,073	5,073						5,073
	Expected run-time per section per seed (min)	2.288E-04	2.185E-04	2.778E-02	2.778E-02	2.778E-02						8.378E-02

All NSAM/NSEED criteria met		Total number of particles at source:	10,200	Minimum sample length/ beam width:	2.903E+00
Estimated total job run time (Settings: Comp. speed relative to benchmark = 1.00):	42 s	Total number of particles at target:	5,073	Maximum sample length/ beam width:	3.193E+01

Scale plot

Legend: — Beam width — Sample length — Sample length / Beam width

Beam Diameter and Sample Length in Total System

Y-axis: Length (m) and Ratio — 1.0E+02, 1.0E+01, 1.0E+00, 1.0E-01, 1.0E-02, 1.0E-03, 1.0E-04

X-axis: z(m) — 0.0E+00, 1.0E-01, 2.0E-01, 3.0E-01, 4.0E-01, 5.0E-01, 6.0E-01, 7.0E-01

Plot scaling parameters	Linear scale (1) or logarithmic scale (2):			2	Reset automatic scaling		NSAM/ NSEED selection	Minimum sample length / minimum beam radius all sections	5.00E+00	==> NSAM_source >		1,664	Suggested setting:	
	Co-ordinate	Min scale	Max scale	Margin %	Min data	Max data		Minimum sample length / maximum beam radius all sections	2.00E+00	==> NSAM_source >		732	NSAM-source	1,700
	Z	0.00E+00	7.20E-01	0%	0.000E+00	7.200E-01	Set to	Minimum sample size at the target	100	==> NSAM_source >		201	NSEED	6
	F(Z)	1.60E-04	3.19E+01	0%	1.600E-04	3.193E+01	default	Minimum total number of particles at the target	5,000	==> NTOT_source >		10,053	NTOT-target	5,073

Worksheet System ('Analytical Model Parameters for Coulomb interaction Effects' section)

Analytical Model Parameters for Coulomb Interaction Effects — Dynam.links: On | On Off

Category	Variable description	Identifier	Unit	1	2	3	4	5	6	7	8	9	10	Target
General properties	Beam current	I	A	1.0000E-05	8.6660E-06	4.9736E-06	4.9736E-06	4.9736E-06						4.9736E-06
	Beam potential at start of section (non-relativistic)	VNR	V	1.0000E+05	1.0000E+05	1.0000E+05	1.0000E+05	1.0000E+05						1.0000E+05
	Acceleration ratio Vend/Vstart (Slice method only)	VRAT	-	1.0000E+00	1.0000E+00	1.0000E+00	1.0000E+00	1.0000E+00						
	Beam section length	L	m	1.6000E-01	1.6000E-01	1.6000E-01	2.0000E-01	4.0000E-02						7.2000E-01
	Distance from start of beam section to physical image plane	LIP	m	3.2000E-01	1.6000E-01	0.0000E+00	2.4000E-01	4.0000E-02						
	Distance from start of beam section to optical image plane	LIO	m	-1.0000E+10	1.6000E-01	0.0000E+00	-1.0000E+10	4.0000E-02						
	Transverse magnification from physical image plane to reference plane	TMP	-	2.5000E-01	2.5000E-01	2.5000E-01	1.0000E+00	1.0000E+00						1.0000E+00
	Transverse magnification from optical image plane to reference plane	TMO		4.0000E-12	2.5000E-01	2.5000E-01	4.0000E-12	1.0000E+00						
	Transverse magnification of section component (lens / quadruple)	TMI	-	1.0000E+00	1.0000E+00	1.0000E+00	2.5000E-01	1.0000E+00						
	Beam type: (1) section with crossover, (2) parallel section	IBT	-	1	2	2	1	1						1
Parameters for beam section with crossover	Crossover position	SC	-	0.0000E+00			8.0000E-01	1.0000E+00						
	Physical image plane position	SIP	-	2.0000E+00			1.2000E+00	1.0000E+00						
	Optical image plane position	SIC	-	-6.2500E+10			-5.0000E+10	1.0000E+00						
	Angular distribution type (1=Uniform, 2=Gauss, 3=Trunc.Gauss, 4=Squa)	IDA0	-	1			4	4						4
	Characteristic beam semi-angle (HWHM)	A0C	Rad	5.0000E-03			3.1250E-03	2.0000E-03						2.0000E-03
	Maximum beam semi-angle (HWHM, used when IDA0=3)	A0M	Rad	5.0000E-03			3.1250E-03	2.0000E-03						2.0000E-03
	Spatial distribution type (1=Uniform, 2=Gauss, 3=Trunc.Gauss, 4=Squar)	IDRC	-	2			2	4						4
	Characteristic crossover radius (HWHM)	RCC	m	8.0000E-05			8.0000E-05	1.2500E-04						1.2500E-04
	Maximum crossover radius (HWHM, used when IDRC=3)	RCM	m	8.0000E-05			8.0000E-05	1.2500E-04						1.2500E-04
Parameters parallel beam section	Spatial distribution type (1=Uniform, 2=Gauss, 3=Trunc.Gauss, 4=Squar)	IDR0	-		4	4								
	Characteristic beam radius (HWHM)	R0C	m		6.9667E-04	5.2500E-04								
	Maximum beam radius (HWHM, used when IDR0=3)	R0M	m		6.9667E-04	5.2500E-04								
	Physical distance to image plane (Focal length)	FLP	m		8.0000E-02	1.6000E-01								
	Optical distance to image plane (Focal length)	FLO	m		8.0000E-02	1.6000E-01								
Model parameters	Include interaction effects in total system evaluation (1=Yes, 0=No)	INT	-	0	0	1	1	1						1
	Interactions correlated to next beam section (1=Yes, 0=No)	ICOR	-	0	1	0	0	0						
	(1) Use analytical formulae; (2) Use slice method	IMETH	-	1	1	1	1	1						

Worksheet System ('Analytical Results for Coulomb interaction Effects' sections)

Analytical Results for Coulomb Interaction Effects

Calculate Coulomb interaction effects by beam section or for all sections ("Calc. All"):					Calculate 1	Calculate 2	Calculate 3	Calculate 4	Calculate 5	Calculate 6	Calculate 7	Calculate 8	Calculate 9	Calculate 10	Calc. All Target
Category	Sub category		Identifier	Unit	Curr.Sec.	1	2	3	4	5	6	7	8	9	10	Target
Coulomb interaction effects	Collapse	Boersch Effect	FWHME	eV	7.6835E-02	2.145E-01	4.840E-02	4.874E-02	2.876E-01	7.683E-02						3.238E-0
	Selected results -		FW50E	eV	5.1663E-02	1.429E-01	3.260E-02	3.283E-02	1.925E-01	5.166E-02						2.169E-0
	Based on:		GamEffE	-	1.5107E+00	1.571E+00	1.501E+00	1.501E+00	1.541E+00	1.511E+00						1.530E+00
	1) IMETH	Trajectory displacement	FWHMR	m	3.1489E-09	6.634E-09	4.464E-09	8.963E-09	2.315E-08	3.149E-09						3.051E-0
	parameter		FW50R	m	5.4414E-09	8.631E-09	5.586E-09	1.125E-08	3.591E-08	5.441E-09						4.568E-0
	2) analytical		d1288R	m	6.1199E-09	9.520E-09	6.179E-09	1.245E-08	3.952E-08	6.120E-09						5.041E-0
	method		d2575R	m	3.1713E-09	5.032E-09	3.260E-09	6.565E-09	2.088E-08	3.171E-09						2.659E-0
	3) slice		GamEffT	-	1.4813E+00	1.527E+00	1.501E+00	1.501E+00	1.578E+00	1.481E+00						1.222E+00
	method	Space charge effect	DZF	m	1.1948E-06	1.094E-06	4.301E-07	1.739E-06	1.633E-05	1.195E-06						2.079E-05
	1		M-1	-	4.8881E-05	-2.568E-04	0.000E+00	0.000E+00	1.465E-04	4.888E-05						-6.150E-05
			CS	m/Rad^3	0.0000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00						0.000E+00

Plots of Analytical Results for Coulomb Interactions from Different Methods and by Beam Section

Also show values for beam sections with INT=0 (INT=0 => Contribution to total effect at target ignored): ☑

Key results from different methods

Contribution by beam section

Analytical Results for Total Energy Spread

Category	Sub category		Identifier	Unit	Source	1	2	3	4	5	6	7	8	9	10	Target
Total energy spread	Selected results for Boersch Effect combined with specified source data		FWHME-BE&S	eV	1.0000E+00	1.000E+00	1.000E+00	1.001E+00	1.052E+00	1.057E+00						1.057E+00
			FW50E-BE&S	eV	5.7285E-01	5.728E-01	5.728E-01	5.739E-01	6.126E-01	6.161E-01						6.161E-0
			GamEffE-BE&S	-	2.0000E+00	2.000E+00	2.000E+00	1.973E+00	1.869E+00	1.847E+00						1.847E+00

Analytical Results for Total Probe Size

Set to default

Category	Sub category	Component	Identifier	Unit	Include ?	Sel.:d2575R	FWHMR	FW50R	d1288R	d2575R	Remarks
Results for total probe size d2575 (m)	Geometrical contributions	Gaussian image	d2575-Gauss	m	☑	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	1) Target is NOT a image of the source: Contribution of Gaussian image ignored
		Diffraction (Airy disk)	d2575-Airy	m	☑	5.8621E-10	9.3724E-10	9.7428E-10	1.0814E-09	5.8621E-10	
		Spherical aberration of lenses	d2575-SpherAb	m	☑	3.4785E-09	7.0988E-09	7.0988E-09	8.2405E-09	3.4785E-09	
		Chromatic aberration from source	d2575-ChromAbSrc	m	☑	8.6680E-10		1.6490E-09	2.0194E-09	8.6680E-10	
	Coulomb interaction effects (selected results)	Chromatic aberration from Boersch effect	d2575-ChromAbBE	m	☑	1.3963E-10		2.6177E-10	3.4566E-10	1.3963E-10	2) Effective beam angle at target used = 2.13E-03 Rad, with a square uniform angular distribution
		Trajectory displacement	d2575-TD	m	☑	2.6585E-08	3.0514E-08	4.5684E-08	5.0411E-08	2.6585E-08	
		Space charge defocus	d2575-DefocusSC	m	☑	1.0000E-15	1.0000E-15	1.0000E-15	1.0000E-15	1.0000E-15	
		Space charge spherical aberration	d2575-SpherAbSC	m	☑	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	
	Totals	Total geometrical aberration disc	d2575-TotalGeom	m	☑	3.5856E-09	7.2883E-09	7.2884E-09	8.4849E-09	3.5856E-09	
		Total Coulomb interaction disc	d2575-TotalInter	m	☑	2.6586E-08	3.0515E-08	4.5685E-08	5.0413E-08	2.6586E-08	
		Total probe size	d2575-Total	m		2.8093E-08	3.4036E-08	4.8815E-08	5.4088E-08	2.8093E-08	

Worksheet Section (top section with collapsed 'Plot Parameters & Key results' view)

| Expand all areas | Collapse all areas | Full Screen On/Off | Unlockcharts | **Beam Section Definition & Calculations** | Increase abs | Decrease abs | 1.000E-06 | Increase % | Decrease % | 1.00% |
| Expand | Collapse | Previous Section | Next Section | At same scale ? □ | **Plots of Key Results for Beam Section 4 - Beam with a Crossover** | | | | | Tune slice parameters |

Geometry of Beam Section 4 / Boersch Effect / Trajectory Displ. Effect / Space charge defocus / Build-Up Interaction Effects in Beam Section (Slice Method)

| Expand | Collapse | **Plot Parameters & Key Results** |
| Expand | Collapse | **Beam Section 4 Input Parameters** |

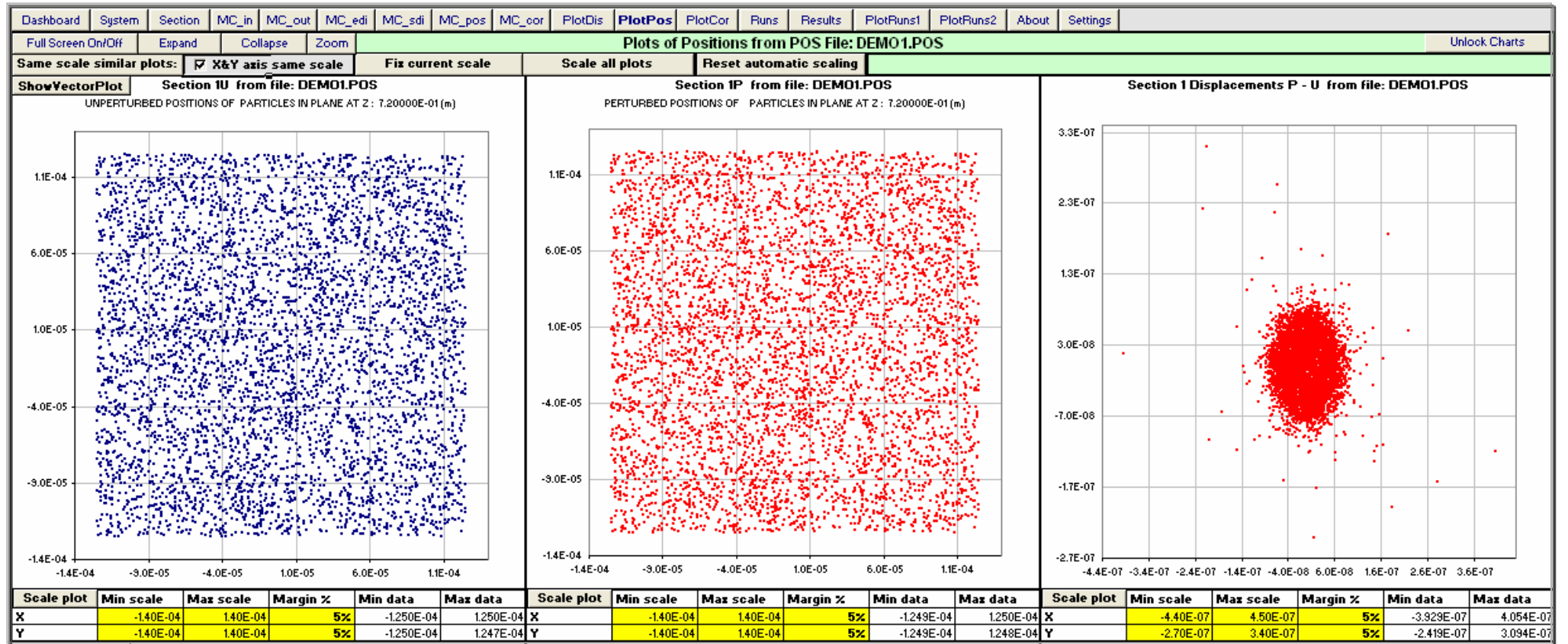|	Category	Description	Symbol	Unit	Input Value	Minimum	Maximum	Remarks on selected input value
Input parameters for beam section	General beam section properties	Beam current	I	A	4.974E-06	1.000E-15		
		Beam potential at start of section (non-relativistic)	VNR	V	1.000E+05	1.000E-15		
		Acceleration ratio Vend/Vstart (Slice method only)	VRAT	–	1.000E+00	1.000E-15		
		Beam section length	L	m	2.000E-01	1.000E-15		
		Transverse magnification from physical image plane to reference plane	TMP	–	1.000E+00	1.000E-15		
		Transverse magnification from optical image plane to reference plane	TMO	–	4.000E-12	1.000E-15		
		Beam type: (1) section with crossover, (2) parallel section	IBT	–	1	1	2	Beam section with crossover
	Input for beam section with a crossover (Input required when IBT=1)	Crossover position	SC	–	8.000E-01	–1.000E+03	1.000E+03	
		Physical image plane position	SIP	–	1.200E+00			
		Optical image plane position	SIO	–	–5.000E+10			
		Angular distribution type (1=Uniform, 2=Gauss, 3=Trunc.Gauss, 4=Square.U	IDA0	–	4	1	4	Square uniform angular distribution in crossover
		Characteristic beam semi-angle (HWHM)	A0C	Rad	3.125E-03	1.000E-15		
		Maximum beam semi-angle (HWHM, used when IDA0=3)	A0M	Rad	3.125E-03	1.000E-15		
		Spatial distribution type (1=Uniform, 2=Gauss, 3=Trunc.Gauss, 4=Square.U	IDRC	–	2	1	4	Gaussian spatial distribution in crossover
		Characteristic crossover radius (HWHM)	RCC	m	8.000E-05	1.000E-15		
		Maximum crossover radius (HWHM, used when IDRC=3)	RCM	m	8.000E-05	1.000E-15		
	Input for parallel beam section (Input required when IBT=2)	Spatial distribution type (1=Uniform, 2=Gauss, 3=Trunc.Gauss, 4=Square.U	IDR0	–		1	4	
		Characteristic beam radius (HWHM)	R0C	m		1.000E-15		
		Maximum beam radius (HWHM, used when IDR0=3)	R0M	m		1.000E-15		
		Physical distance to image plane (Focal length)	FLP	m		0.000E+00		
		Optical distance to image plane (Focal length)	FLO	m		0.000E+00		
	Relation between beam section and total system specification	Beam section number	ISEC	–	4	1	10	
		Include interaction effects in total system evaluation (1=Yes, 0=No)	INT	–	1	0	1	Interaction effects included in system calculation
		Interactions correlated to next beam section (1=Yes, 0=No)	ICOR	–	0	0	1	Interactions independent from other sections
	Model selection	(1) Use analytical formulae; (2) Use slice method	IMETH	–	1	1	2	Use analytical formulae

Worksheet Section ('Calculated Theoretical Parameters" and 'Calculated interaction Effects' sections)

Calculated Theoretical Parameters

	Category	Description	Symbol	Unit	Result	Category	Description	Symbol	Unit	Result
Calculated theoretical Parameters	General	Beam potential	V	V	1.000E+05	For beam section	v0-d0 scales	v_0	m/s	6.613E+05
		Relativistic beam potential	$V_{relativistic}$	V	1.098E+05	with crossover		d_0	m	5.790E-10
		Axial velocity	v_z	m/s	1.876E+08		Effective beam semi-angle	$\alpha_{0,eff}$	Rad	3.526E-03
		Axial velocity / light speed	v_z/c	-	6.256E-01		Effective crossover radius	$r_{c,eff}$	m	9.609E-05
		Linear particle density	λ	1/m	1.655E+05		Reduced brightness	β_r	A / (m^2 Sr V)	4.389E+01
		Average axial separation	$1/\lambda$	m	6.042E-06		Scaled linear particle density (Lambda-bar)	$\bar{\lambda}$	-	9.584E-05
		v–δ scales	v	m/s	9.831E+03		Pencil beam factor for beam with crossover	$\mathfrak{X}_C$	-	1.167E+02
			δ	m	1.048E-05		Characteristic beam geometry quantities	K	-	3.670E+00
	For parallel beam section	Effective beam radius	$r_{0,eff}$	m				K_1	-	5.871E+00
		Reduced current density	J_r	A / (m^2 V)				K_2	-	1.468E+00
		Scaled linear particle density (Lambda-star)	$\bar{\lambda}^*$	-			Scaled crossover radius (RC-bar)	$r_c\bar{}$	-	1.659E+05
		Pencil beam factor for parallel beam	$\mathfrak{X}_P$	-			Scaled crossover radius (RC-star)	r_c^*	-	9.166E+00
		Scaled beam radius (R0-star)	r_0^*	-			Scaled characteristic transverse velocity (V0-star)	v_0^*	-	6.727E+01

Calculated Interaction Effects

	Category	Description	Symbol	Unit	Selected	Analytical	Slice meth.
Calculated Coulomb interaction effects	Boersch Effect	FWHM energy spread	FWHME	eV	2.876E-01	2.876E-01	2.081E-01
		FW50 energy spread	FW50E	eV	1.925E-01	1.925E-01	1.401E-01
		Effective γ–value energy distribution	GamEffE	-	1.541E+00	1.541E+00	1.507E+00
	Angular deflection	FWHM angular displacement distribution width	FWHMA	Rad	2.199E-06	2.199E-06	2.772E-07
		FW50 angular displacement distribution width	FW50A	Rad	3.110E-06	3.110E-06	3.490E-07
		d1288 angular displacement distribution edge width	D1288A	Rad	3.185E-06	3.185E-06	3.861E-07
		d2575 angular displacement distribution edge width	D2575A	Rad	3.115E-06	3.115E-06	2.037E-07
		Effective γ–value angular displacement distribution	GamEffA	-	1.903E+00	1.903E+00	1.501E+00
	Trajectory displacement	FWHM trajectory displacement distribution width	FWHMR	m	2.315E-08	2.315E-08	1.109E-08
		FW50 trajectory displacement distribution width	FW50R	m	3.591E-08	3.591E-08	1.396E-08
		d1288 trajectory displacement distribution edge width	d1288R	m	3.952E-08	3.952E-08	1.544E-08
		d2575 trajectory displacement distribution edge width	d2575R	m	2.088E-08	2.088E-08	8.147E-09
		Effective γ–value trajectory displacement distribution	GamEffT	-	1.578E+00	1.578E+00	1.501E+00
	Space charge effect	Space charge axial defocus distance	DZF	m	1.633E-05	1.633E-05	6.735E-05
		Space charge induced change in magnification	M-1	-	1.465E-04	1.465E-04	0.000E+00
		Space charge induced spherical aberration	CS	m/Rad^3	0.000E+00	0.000E+00	2.655E-07

Worksheet PlotDis
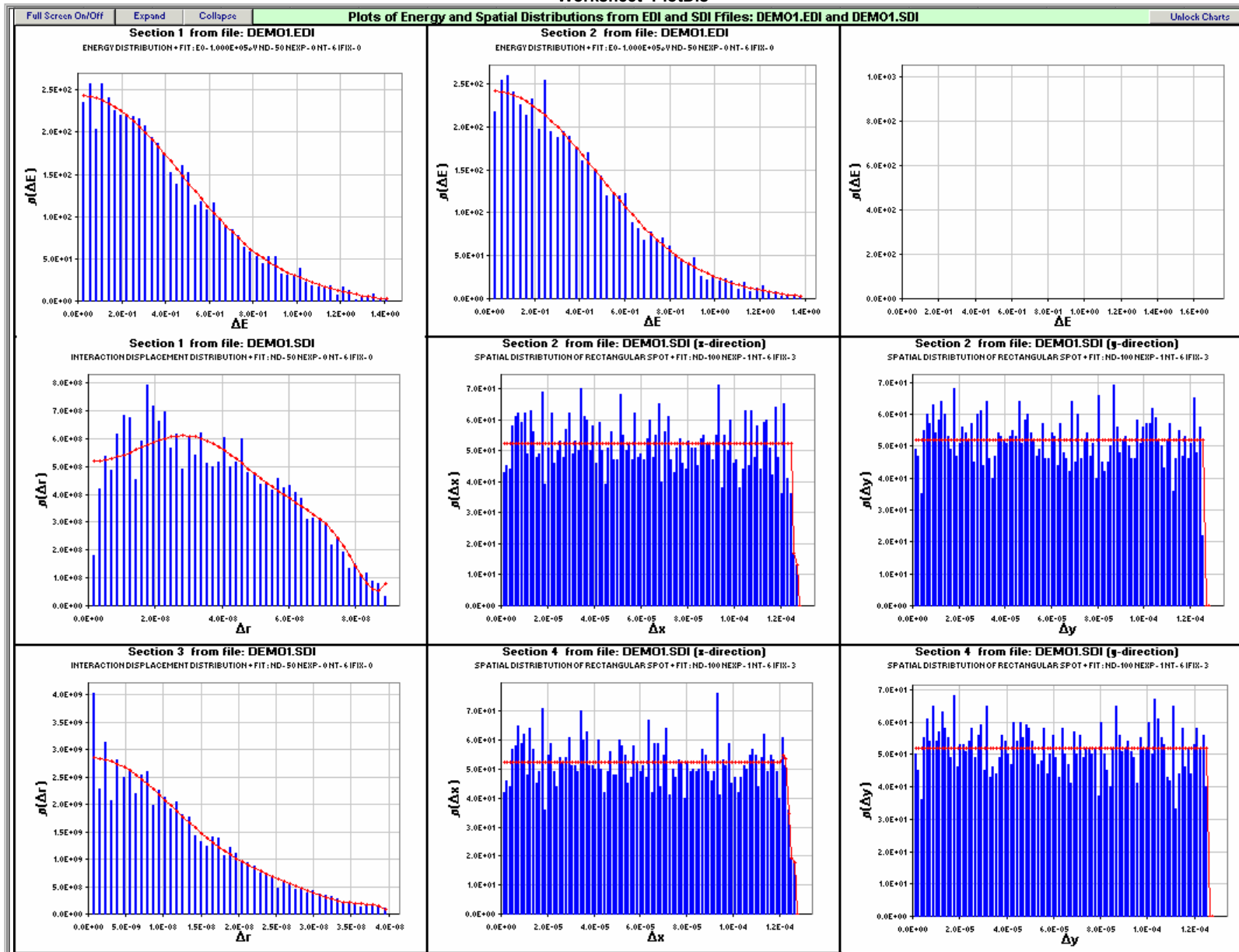
Worksheet PlotPos (Top section)

Worksheet PlotCor (Graphs row 3 and 4)

Worksheet PlotCor (Graphs row 5 and 6)

From file: DEMO1.COR
Unperturbed lateral velocities

From file: DEMO1.COR
Perturbed lateral velocities

From file: DEMO1.COR
Lateral velocity displacements

From file: DEMO1.COR
Histogram of unperturbed lateral velocities

From file: DEMO1.COR
Histogram of perturbed lateral velocities

From file: DEMO1.COR
Histogram of lateral velocity displacements
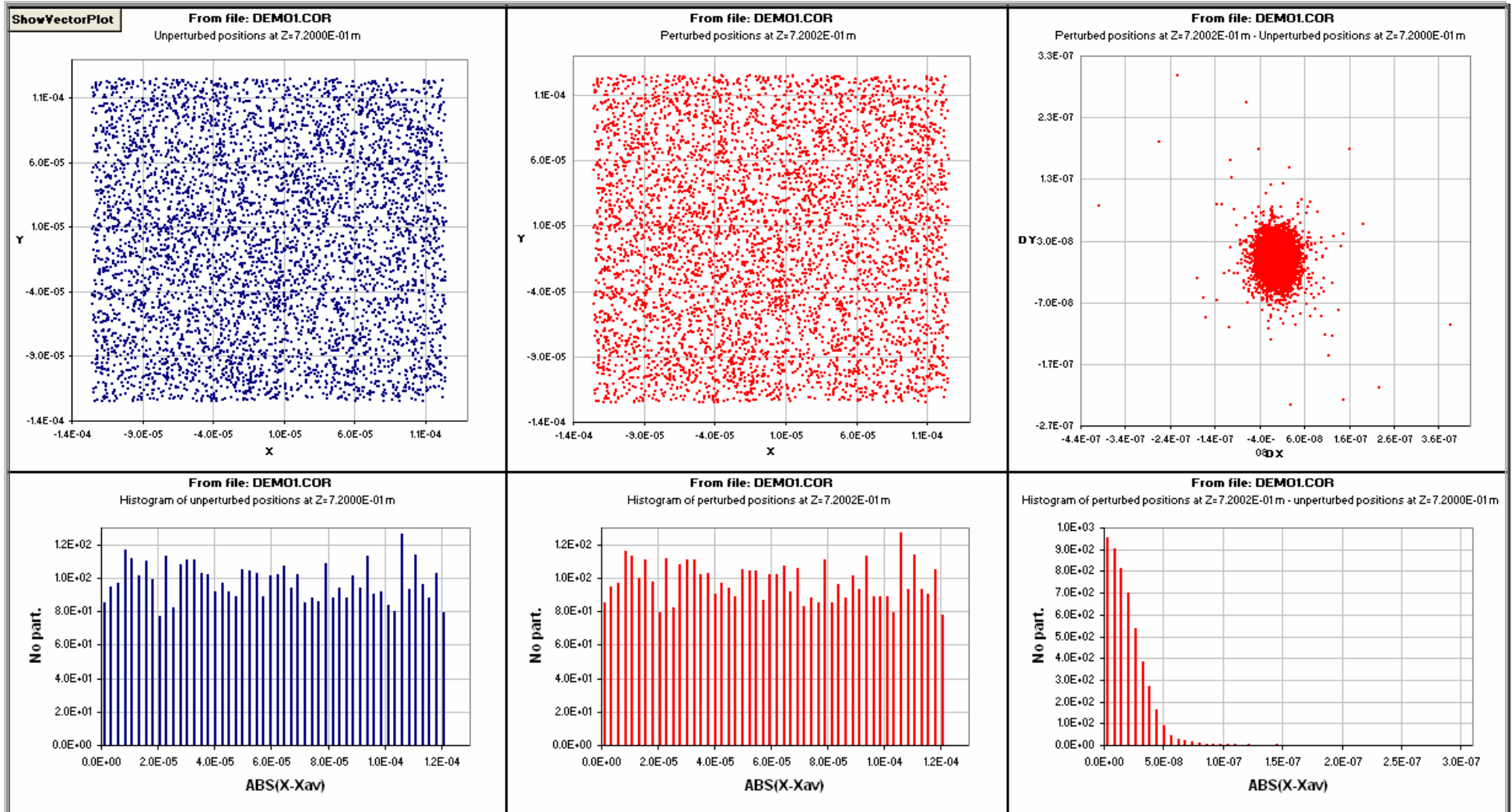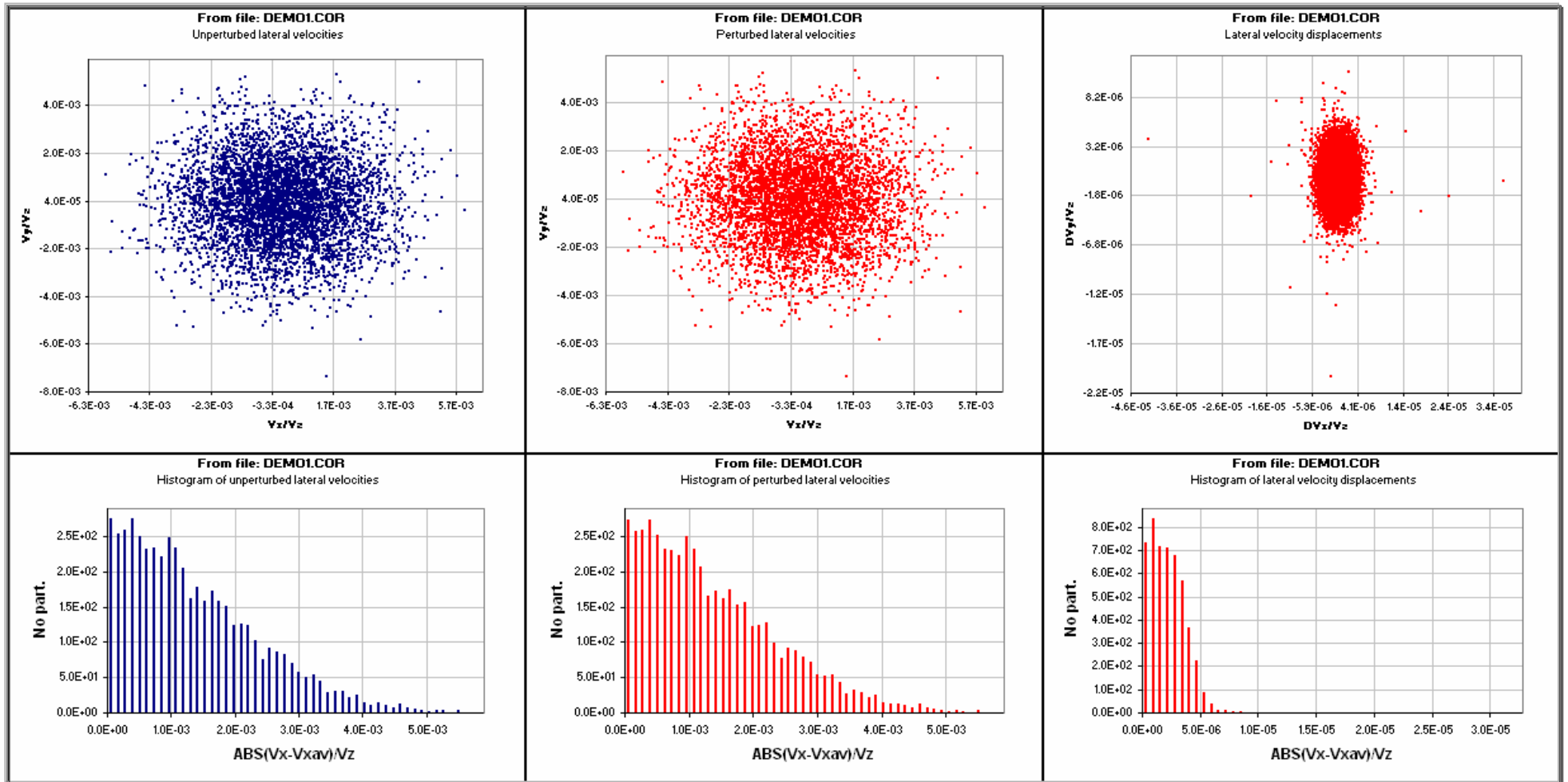
Worksheet PlotCor (Vector plot window)

Worksheet PlotRuns1

Plot Results of Selected Runs – Labeled X-axis

Test results Boersch effect — FW50E-BP, FW50E-AP, FW50E-I&S

Test results traj. displ. effect and defocus — FW50R-BF, FW50R-AF, FW50R-IA, DZF-MC, DZF-IA

Test results run time — MC run time-MC, MC run time est.-IA

Specify Plot Data through 'Results' Row Index

X-Axis	Used labels		2	3	4	5	6	7	8
Chart 1	33	FW50E-BP	1.427E+00	2.377E+00	3.008E+00	3.193E+00	2.614E+00	1.957E+00	1.458E+00
Y-Axis data	35	FW50E-AP	7.935E-01	9.142E-01	9.882E-01	1.026E+00	1.083E+00	1.162E+00	1.123E+00
from Results	88	FW50E-I&S	1.135E+00	1.135E+00	1.135E+00	1.135E+00	1.135E+00	1.135E+00	1.135E+00
worksheet			1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15
Add tag ? ☑			1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15
Chart 2	41	FW50R-BF	2.458E-07	4.417E-07	6.076E-07	7.508E-07	8.714E-07	9.276E-07	9.797E-07
Y-Axis data	44	FW50R-AF	1.237E-07	1.700E-07	1.998E-07	2.245E-07	2.327E-07	2.305E-07	2.304E-07
from Results	91	FW50R-IA	1.955E-07	2.057E-07	1.955E-07	2.057E-07	1.955E-07	2.057E-07	2.057E-07
worksheet	46	DZF-MC	4.256E-05	9.025E-05	1.337E-04	1.703E-04	1.921E-04	2.032E-04	2.055E-04
Add tag ? ☑	105	DZF-IA	2.079E-04	2.208E-04	2.079E-04	2.208E-04	2.079E-04	2.208E-04	2.208E-04
Chart 3	66	MC run time-MC	4.333E-01	8.500E-01	1.100E+00	1.567E+00	3.433E+00	7.400E+00	1.358E+01
Y-Axis data	158	MC run time est.-	5.746E-01	7.011E-01	9.727E-01	1.539E+00	3.254E+00	6.120E+00	1.185E+01
from Results			1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15
worksheet			1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15
Add tag ? ☑			1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15

Worksheet PlotRuns1

System results Boersch effect

System results trajectory displacement effect

System results space charge defocus

X-Axis	Used:	ITARGET-MC	5.000E-07	2.500E-06	2.500E-06	4.986E-06	9.973E-06	2.465E-05	4.989E-05
Chart 1	33	FW50E-BP	5.692E-01	5.931E-01	5.931E-01	6.242E-01	6.950E-01	9.908E-01	1.421E+00
Y-Axis data	35	FW50E-AP	5.684E-01	5.927E-01	5.927E-01	6.127E-01	6.598E-01	8.483E-01	1.120E+00
from Results	79	FW50E-IA	4.738E-02	1.376E-01	1.376E-01	2.169E-01	3.409E-01	6.149E-01	9.536E-01
worksheet	88	FW50E-I&S	5.748E-01	5.901E-01	5.901E-01	6.161E-01	6.755E-01	8.588E-01	1.135E+00
Add tag ? ☑			1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15
Chart 2	41	FW50R-BF	1.093E-08	5.337E-08	5.337E-08	1.033E-07	2.008E-07	4.879E-07	9.821E-07
Y-Axis data	44	FW50R-AF	6.321E-09	2.298E-08	2.298E-08	3.860E-08	6.442E-08	1.309E-07	2.300E-07
from Results	91	FW50R-IA	9.401E-09	2.894E-08	3.051E-08	4.807E-08	7.509E-08	1.339E-07	2.057E-07
worksheet			1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15
Add tag ? ☑			1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15
Chart 3	46	DZF-MC	1.515E-06	8.870E-06	8.870E-06	1.836E-05	3.884E-05	1.001E-04	2.101E-04
Y-Axis data	105	DZF-IA	2.079E-06	1.040E-05	1.104E-05	2.208E-05	4.416E-05	1.104E-04	2.208E-04
from Results			1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15
worksheet			1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15
Add tag ? ☑			1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15	1.000E-15